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6 TEMPERATURE DEPENDENCE OF GAS PROPERTIES IN POLYNOMIAL FORM,

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electronic calculators. Using the polynomial approximations and a suitable calculator, it is possible to duplicate existing reference source tabular values directly, obviating the need for interpolation or further reference to the tables per se. The accuracy of the calculated values can be within 0.5% of the tabular values. The polynomial coefficients are given in the International System of Units (SI). Methods are presented to calculate the temperature corresponding to a given property value. Extrapolation features of the polynomials are discussed.

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# ABSTRACT

Based on a least-squares polynomial approximation, a procedure is introduced for calculating existing tabular values of thermodynamic and transport properties for common gases. The specific heat at constant pressure is given for 238 gases, the thermal conductivity for 55 gases, the dynamic viscosity for 58 gases, and the second and third virial coefficients for 14 gases. At sufficiently low pressures, ideal gas behavior prevails and temperature may be used as the single independent variable. The algorithm for nested multiplication is presented, optimized for hand-held or desktop electronic calculators. Using the polynomial approximations and a suitable calculator, it is possible to duplicate existing reference source tabular values directly, obviating the need for interpolation or further reference to the tables per se. The accuracy of the calculated values can be within 0.5% of the tabular values. The polynomial coefficients are given in the International System of Units (SI). Methods are presented to calculate the temperature corresponding to a given property value. Extrapolation features of the polynomials are discussed.

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## I. INTRODUCTION

Many important thermodynamic and transport properties of gaseous elements and compounds can be expressed purely and accurately as functions of temperature. The perfect gas behavior of simple compressible substances is a well documented example<sup>1-3</sup>. Data tables for such single-variable functions may be approximated with curve-fitting techniques reducing the tabular information to polynomial or exponential forms. Given these equations and a handheld or desktop electronic calculator, a user may retrieve the tabular information accurately and conveniently without interpolation or further reference to the original data sources. The objective of this work is to provide sufficiently simple polynomial fits which together with a modern electronic calculator present the most convenient method of handling the calculation of thermodynamic properties accurately. In all but the most detailed numerical work, the information presented here should prove to be advantageous over present tabular, graphical, or other methods. This report significantly expands the scope of our earlier work<sup>4</sup> by including basic properties of a large number of elements and compounds.

The gas properties for which polynomial equations are presented comprise the specific heat at constant pressure [ $C_p(T)$ ] for 238 gases in Appendix A, the thermal conductivity [ $k(T)$ ] for 55 gases in Appendix B, the dynamic viscosity [ $\mu(T)$ ] for 58 gases in Appendix C, and the second and third virial coefficients for 14 gases in Appendix D. The accuracy of reproduction of source data is within 0.5%. The correlating equations are presented in the International System of Units (SI). To further enhance the usefulness of this work, methods are given to reverse the dependent and independent variables (i.e., to calculate the temperature corresponding to a given property

value); these methods consist of either polynomials for the inverse calculation as given in the Appendixes or the iterative procedures discussed in Section 5.

In any effort such as this, consideration must be given to the range of validity of the polynomial fit in addition to its accuracy. Section 2 addresses these important topics. The possibility and limitation of extrapolation is discussed in Section 4. Also, the technique of nested multiplication is discussed in Section 3; this technique is a "natural" for the majority of electronic calculators presently available and provides for the convenient use of the information presented herein.

It should be noted that for a perfect or ideal gas (with variable heat capacities) having  $C_p$  in polynomial form is particularly useful. This is because the polynomials may be integrated easily, without risking any decrease in the accuracy of the results. The well known relations for a perfect or ideal gas are summarized below and Ref. 5 expands on the technique for generating the gas tables.

$$C_v = C_p - R \quad [\text{specific heat at constant volume}]$$

$$\gamma = C_p / (C_p - R) \quad [\text{ratio of heat capacities}]$$

$$h = \int C_p dT \quad [\text{enthalpy}]$$

$$u = h - RT \quad [\text{internal energy}]$$

$$\phi = \int C_p \frac{dT}{T} \quad [\text{entropy function}]$$

While the simplicity and utility of the perfect or ideal gas calculations is readily apparent, imperfect or real gas behavior is also important. In the Appendixes, therefore, two headings are often found, i.e., ideal gas and real gas. We also include in this work polynomial fits for the second



and third virial coefficients. These allow accurate representation of non-ideal behavior at densities as high as 0.7 of the critical value<sup>6</sup>.

The material in this report is intended to be used in conjunction with standard reference texts on thermodynamics, fluid dynamics, and heat transfer. The user is encouraged, moreover, to discover for himself how the simple polynomial fits aid in the handling of differential equations with variable coefficients.

## II. POLYNOMIAL CURVE FITS

The data source for Appendixes A, B, and C is the TRPC<sup>7-9</sup> series. The virial coefficients are found in the American Institute of Physics Handbook, 3rd Edition<sup>10</sup>. These sources are considered to be among the most accurate. The TRPC series reproduce a large number of original sources and present a critically evaluated consolidation of available data. The accuracy of duplication of reference-source values is included with the polynomial equations as part of the format in the Appendixes [see pp. A-viii, B-iii, C-iii, and Di1]. References 7-9 include their own third-degree polynomial fits; other polynomial expressions are also available<sup>11,12</sup> in most thermodynamic textbooks.

The most important consideration given in the curve fitting is the reliability of the data. Next to reliability, consideration is given to the greatest possible temperature range; reference source data are split along temperature intervals to achieve the most acceptable duplication accuracy. The equations presented are the lowest degree equations which achieve the desired accuracy over the temperature range stated.

### III. POLYNOMIAL EVALUATIONS

For the calculation of properties or the inverse calculation of the temperature, we have relied almost exclusively on polynomial fits, with the exception of some specific heat [ $C_p(T)$ ] forms which are exponential. The equations presented have the following forms:

#### Polynomial

$$FCTN(T) = B(0) + B(1)T + B(2)T^2 + \dots + B(N)T^N = \sum_{m=0}^N B(m)T^m$$

#### Exponential

$$\ln[FCTN(T)] = B(0) + B(1)T + \dots + B(N)T^N = \sum_{m=0}^N B(m)T^m$$

$$[e.g., C_p(T) = (\text{const}) \exp \left[ \sum_{m=0}^N B(m)T^m \right]]$$

The most efficient method of evaluating single-variable polynomials is "nested multiplication"<sup>13</sup>. Nested multiplication eliminates the need to raise "X" to the "Y" power and simplifies an N-th order polynomial evaluation to a sequence of multiplication/addition steps. Examples of nested multiplication are presented below.

#### A. Generalized Nested Multiplication Algorithm:

Given the N coefficients,  $B(0), B(1), B(2), \dots, B(N)$ , for the polynomial function  $FCTN(T)$  and any value of the temperature " $T_i$ " within the range of validity

Set  $A(N) = B(N)$  [e.g.,  $A(6) = B(6)$ ]

For  $K = N, N-1, N-2, \dots, 1$ , Do

Set  $A(K-1) = B(K-1) + T_i A(K)$

$A(0) = FCTN(T_i)$

The above algorithm may be stated in words as follows: multiply the highest degree coefficient by the temperature value,  $T_1$ , and add to the next lower degree coefficient; multiply the sum by  $T_1$  and add to the next lower degree coefficient; multiply the sum by  $T_1$  ... Continue the process until the sum  $B(1)+A(2)T_1$  is calculated; multiply this sum by  $T_1$ . By just adding the  $B(0)$  coefficient to the previous product, the polynomial evaluation is completed for the chosen value of  $T_1$ .

B. Specific Example of Nested Multiplication:

Consider the calculation of the specific heat at constant pressure  $[C_p(T)]$  for carbon dioxide ( $CO_2$ ), ideal gas, at  $800^\circ K$ . From page A-9,

$$C_p(T) = 453.86462 + 1.5334795T - 4.195556E-04 T^2 \\ - 1.871946E-06 T^3 + 2.862388E-09 T^4 \\ - 1.6962E-12 T^5 + 3.717285E-16 T^6$$

$$\text{Set } A(6) = 3.717285E-16 ; T = 800$$

Step-by-Step Procedures			Calculated Values	A(N)
(1)	3.717285E-16	B(6) =	3.717285E-16	A(6)
(2)	X800	$XT_1$	2.973828E-13	
(3)	-1.6962E-12	+B(5)	-1.3988172E-12	A(5)
(4)	X800	$XT_1$	-1.11905376E-09	
(5)	+2.862388E-09	+B(4)	1.74333424E-09	A(4)
(6)	X800	$XT_1$	1.394667392E-06	
(7)	-1.871946E-06	+B(3)	-4.77278608E-07	A(3)
(8)	X800	$XT_1$	-3.818228864E-04	
(9)	-4.195556E-04	+B(2)	-8.013784864E-04	A(2)
(10)	X800	$XT_1$	-0.641102789	
(11)	+1.5334795	+B(1)	0.892376711	A(1)
(12)	X800	$XT_1$	713.9013687	
(13)	+453.86462	+B(0)	1167.765989	A(0)

Rounding to two decimal places,  $A(0) = C_p(800K) = 1167.77 \text{ J/Kg K}$ .

For programmable calculators, nested multiplication is extremely efficient and highly recommended. To preserve the add-multiply-add simplicity, negative coefficients should be stored as negative values.

#### IV. EXTRAPOLATION

With each polynomial equation there is a specified range of validity and an associated error estimate. The stated temperature range corresponds to that of the reference source. It is often highly desirable to know how the given polynomial expressions extrapolate. A limited polynomial extrapolation beyond the specified temperature range may often be possible but in indiscriminate extrapolation the accuracy will most likely suffer. In fact, polynomial fits are notoriously bad for certain type of curves outside of their specified range.

Clearly, it is inappropriate to look at every possible type of variation. Suffice it to say that for reasonably smooth, monotonic functions such as the viscosity, the thermal conductivity, and perhaps the heat capacity of polyatomic molecules, the polynomial fits will follow with some fidelity the trends outside of their specified range. If is anticipated that the heat capacity of diatomic molecules will be the most difficult for the polynomials to follow because of the "stepwise" nature of the curves<sup>14,15</sup>. We have chosen to present the heat capacity of nitrogen as an example. The ideal gas polynomial fits are given on pg. A-41; we choose the curve for the temperature range 590-1365°K. As the basis of comparison, we pick the theoretical<sup>14</sup> curve which represents the activation of the vibrational mode of the nitrogen molecule, using  $\theta_v = 3390^\circ\text{K}$ . Table I shows a listing of these calculations. It is seen that the polynomial results are within an acceptable  $\pm 0.5\%$  for the temperature range 500°K to 1600°K. Above and below this range the polynomial results quickly diverge as more or less anticipated. Certainly, a useful rule may be to stay within 100°K of the guaranteed range.

TABLE I

POLYNOMIAL COMPARISON,  $C_p$  FOR NITROGEN

T (K)	CP/R THEO	CP/R POLY	%DIFF
400	3.51513	3.55253	-1.06371
500	3.55272	3.56516	- .35014
600	3.6137	3.62092	- .199842
700	3.68868	3.69739	- .236274
800	3.76795	3.77981	- .314853
900	3.84486	3.85952	- .381236
1000	3.91588	3.9325	- .424339
1100	3.97859	3.99775	- .456325
1200	4.03582	4.05591	- .497772
1300	4.08501	4.10757	- .552173
1400	4.12787	4.15159	- .574591
1500	4.16518	4.18432	- .45953
1600	4.19768	4.19665	.024718
1700	4.22606	4.17417	1.22786
1800	4.2509	4.09448	3.67977

The reader might ask at this point why bother with a polynomial when an exact expression is available. The answer to this question is two-fold: First, reliable analytical expressions are not available for most of the properties and, second, when available they tend to be much more cumbersome than the polynomial expressions presented here.



## V. ITERATIVE METHODS

It is often necessary to calculate the temperature from the known value of a property. This inverse problem is handled two ways, either a polynomial fit is given in Appendixes A, B, and C for the calculation of the absolute temperature as a function of the property or an iterative procedure is suggested. In this section we discuss such iterative methods.

Before proceeding, however, it is worth noting that when a second degree polynomial in  $T$  is given for the inverse calculation, the quadratic formula may be applied. If it works, this is by far the quickest way to a solution.

The polynomials presented have the absolute temperature ( $T$ ) as the single independent variable and the property value ( $PV$ ) as the dependent variable.  $FCTN(T_i)$  becomes the magnitude of the property value ( $PV$ ) when the polynomial function is evaluated at  $T = T_i$ . Thus,  $FCTN(T_i) = |PV|$  at  $T = T_i$ . To enhance the usefulness of this work, three methods are provided for the calculation of temperature ( $T$ ) as a function of a known or given property value,  $PV$ . The methods are (A) secant method, (B) Newton's method, and (C) fixed point iteration<sup>16</sup>. All three methods are iterative in nature.

The general form of the polynomials is

$$FCTN(T_i) = B(0) + B(1)T_i + B(2)T_i^2 \dots B(N)T_i^N$$

The iterative methods attempt to solve for the approximate root (the temperature) of the equation of the form

$$F(T_i) = PV - B(0) - B(1)T_i - B(2)T_i^2 \dots - B(N)T_i^N = 0$$

All of the polynomials are both continuous and continuously differentiable over the temperature intervals specified. Although these conditions are necessary for iterative methods to converge to an approximate root,

they are not necessarily sufficient in all cases to assure convergence. Enough testing has been done with the polynomials presented, however, to given reasonable assurance of convergence with any of the three methods discussed.

The quadratic formula for the second degree polynomial is simply

$$T = \frac{-B(1) + \sqrt{B(1)^2 - 4 B(2)[B(0) - PV]}}{2 B(2)}$$

A. Secant or Interpolation Method<sup>13,16</sup>:

When it converges, the secant method does so very rapidly, generally more rapidly than either of the other two iterative methods discussed. Two initial values (guesses) for the temperature are required,  $T_{-1}$  and  $T_0$ . The initial temperature values selected may be the extremes of the valid temperature range noted with the polynomial sets.

Algorithm: Given  $(T_i) = 0$  and two (2) initial points,  $T_{-1}$  and  $T_0$

For  $n = 0, 1, 2, \dots$  until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - F(T_n) \frac{(T_n - T_{n-1})}{F(T_n) - F(T_{n-1})}$$

In the special case when second degree polynomials given in the Appendix, the secant method algorithm reduces to:

For  $n = 0, 1, 2, \dots$  until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - \frac{B(0) + B(1)T_n + B(2)T_n^2 - (PV)}{B(1) + B(2)(T_n + T_{n-1})}$$

Specific Example: Consider a second (2nd) degree polynomial for  $C_p(T)$ :  $FCTN(T_i) = 0.232829 + 1.43429E-05T_i + 3.56638E-09T_i^2$ . Assume a given property value  $C_p = 0.2567$  but the temperature is unknown. The

known property value (PV) is 0.2567 and  $T_{-1}$  and  $T_0$  are chosen arbitrarily at 200 and 2400 respectively. The following solution is provided:

n	$T_{n-1}$	$T_n$	$T_{n+1}$
0	200	2400	-
1	2400	2400	1411.67
2	2400	1411.67	1286.97
3	1411.67	1286.97	1266.32
4	1286.97	1266.32	1265.87
5	1266.32	1265.87	1265.87* Convergence

$$T_1 = 1265.87 \text{ for } C_p(T_1) = 0.2567$$

#### B. Newton's Method<sup>16</sup>:

Newton's method requires a single initial value for temperature,  $T_0$ , and the first derivative of the polynomial function,  $F(T_1) = 0$ . Newton's method tends to be sensitive to the  $T_0$  selection, the closer  $T_0$  is to the root,  $T_1$ , the more rapid it converges. For the polynomials presented, Newton's method generally converges without problems. It is recommended that the initial temperature value,  $T_0$ , be selected mid-range between the polynomial valid temperature limits.

Algorithm: Given  $F(T_1) = 0$  and a starting value,  $T_0$

For  $n = 0, 1, 2, \dots$  until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - F(T_n)/F'(T_n)$$

For the special case of using a second degree polynomial from

Appendix A, Newton's method reduces to the following:

For  $n = 0, 1, 2, \dots$  until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - \frac{B(0) - (PV) + B(1)T_n + B(2)T_n^2}{B(1) + 2B(2)T_n}$$

C) Fixed Point Iteration:<sup>16</sup>

Fixed point iteration tends to converge the slowest of the three methods discussed. It does, however, provide the user with the function definition. Given the function,  $F(T_1) = 0$ , the user defines an iterative function,  $T = g(T_1)$ , such that the solution of the iterative function is also the solution to  $F(T_1) = 0$ .

Example: Given  $F(T_1) = 0 = B(0) + B(1)T_1 + B(2)T_1^2 - (PV)$

$$\text{Then } T_1 = g_1(T) = \frac{(PV) - B(2)T_1^2 - B(0)}{B(1)}$$

$$\text{Or } T_1 = \left( \frac{(PV) - B(0) - B(1)T_1}{B(2)} \right)^{1/2}$$

Algorithm: Given  $F(T_1) = 0$ , a derived iterative function  $g(T)$ , and a single starting point,  $T_0$

For  $n = 0, 1, 2, \dots$  until satisfied, do

Calculate  $T_{n+1} = g(T_n)$

## VI. CONCLUSIONS

Within the constraints of a single independent variable (the absolute temperature), it is possible to calculate thermodynamic and transport properties of a large variety of gases accurately. The accuracy of the polynomial results is generally within  $\pm 0.5\%$  of the original tabular data. Since interpolation is "build-in", the effort is often no more time consuming than that of reading conventional tabular forms. The inverse problem, namely that of finding the temperature corresponding to a given property, can also be accurately carried out with the information given in this report.

Extrapolation beyond the established valid temperature range is possible but the accuracy of duplication of the property is dubious and cannot be quantified in most cases. The polynomials, however, do allow for a convenient "first guess" in most instances.

It is believed that the combination of simple polynomial representations with the technique of nested multiplication utilized in a modern electronic calculator will make the Gas Tables and other standard works obsolete in form. Integration and differentiation of the polynomials is, moreover, straightforward and virtually risk free so that they are attractive forms for numerical work, particularly with ideal gases. The advantages of simple polynomial representations become vividly clear when other correlation-equation forms are used, see for example the form of the viscosity given in Ref. 5 or 17.

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APPENDIX A  
TABLE A-I  
SUMMARY OF CONTENTS

SPECIFIC HEAT AT CONSTANT PRESSURE  
FOR GASEOUS ELEMENTS AND COMPOUNDS

NAME	FORMULA	AT.WT/ MOL WT	GAS CONST	APP A PAGE
Acetone	C <sub>3</sub> H <sub>6</sub> O	58.081	143.150	A-1
Acetylene	C <sub>2</sub> H <sub>2</sub>	26.038	319.312	A-1
Air	-	28.966	287.037	A-1
Ammonia	NH <sub>3</sub>	17.031	488.199	A-2
Argon	Ar	39.948	208.129	A-2
Arsine	AsH <sub>3</sub>	77.946	106.668	A-2
Arsine, Trideuterated	AsD <sub>3</sub>	80.964	102.692	A-2
Benzene	C <sub>6</sub> H <sub>6</sub>	78.115	106.437	A-3
Boron Fluoride Oxide, Trimeric	(BOF) <sub>3</sub>	137.426	60.500	A-3
Boron Tribromide	BBr <sub>3</sub>	250.538	33.186	A-3
Boron Trichloride	BCl <sub>3</sub>	117.170	70.959	A-4
Boron Trifluoride	BF <sub>3</sub>	67.806	122.619	A-4
Bromine	Br <sub>2</sub>	159.818	52.024	A-4
Bromine (Monatomic)	Br	79.909	104.047	A-5
Bromine Chloride	BrCl	115.362	72.072	A-5
Bromine Fluoride	BrF	98.907	84.062	A-5
Bromine Pentafluoride	BrF <sub>5</sub>	174.901	47.537	A-5
Bromoform	CHBr <sub>3</sub>	252.746	32.896	A-5
Bromomethane	CH <sub>3</sub> Br	94.944	87.571	A-6
Bromotrichloromethane	CCl <sub>3</sub> Br	198.279	41.932	A-6
1,3-Butadiene	(CH <sub>2</sub> CH) <sub>2</sub>	54.092	153.706	A-6
iso-Butane	i-C <sub>4</sub> H <sub>10</sub>	58.124	143.044	A-6
n-Butane	n-C <sub>4</sub> H <sub>10</sub>	58.124	143.044	A-7
1-Butanol	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> OH	74.124	112.168	A-7
2-Butanone	CH <sub>3</sub> CH <sub>2</sub> COCH <sub>3</sub>	72.108	115.304	A-7
1-Butene	CH <sub>2</sub> CHCH <sub>2</sub> CH <sub>3</sub>	56.108	148.183	A-7
2-Butene	(CH <sub>3</sub> CH) <sub>2</sub>	56.108	148.183	A-8
cis-2-Butene	(CH <sub>3</sub> CH) <sub>2</sub>	56.108	148.183	A-8
trans-2-Butene	(CH <sub>3</sub> CH) <sub>2</sub>	56.108	148.183	A-8
Butyl Ether	[CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> ] <sub>2</sub> O	130.232	63.842	A-8
1-Butyne	CHCCH <sub>2</sub> CH <sub>3</sub>	54.092	153.706	A-8
2-Butyne	(CH <sub>3</sub> C) <sub>2</sub>	54.092	153.706	A-9
Carbon (Atomic)	C	12.0112	*692.217	A-9
Carbon Dioxide	CO <sub>2</sub>	44.010	188.919	A-9
Carbon Disulfide	CS <sub>2</sub>	76.139	109.199	A-10
Carbon Monoxide	CO	28.011	296.828	A-10
Carbon Monosulfide	CS	44.075	188.640	A-10

\*Atomic weight of carbon is 12.01115



TABLE A-I  
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Carbon Suboxide	C <sub>3</sub> O <sub>2</sub>	68.032	122.211	A-10
Carbon Tetrabromide	CBr <sub>4</sub>	331.647	25.070	A-10
Carbon Tetrachloride	CCl <sub>4</sub>	153.823	54.051	A-11
Carbonyl Chloride Fluoride	COClF	82.462	100.826	A-11
Carbonyl Fluoride	COF <sub>2</sub>	66.007	125.961	A-11
Carbonyl Sulfide	COS	60.075	138.400	A-11
Chlorine	Cl <sub>2</sub>	70.906	117.258	A-12
Chlorine (Monatomic)	Cl	35.453	234.517	A-12
Chlorine Dioxide	ClO <sub>2</sub>	67.452	123.263	A-12
Chlorine Fluoride	ClF	54.451	152.692	A-12
Chlorine Monoxide	Cl <sub>2</sub> O	86.905	95.671	A-13
Chlorine Oxide	ClO	51.452	161.592	A-13
Chlorine Trifluoride	ClF <sub>3</sub>	92.448	89.935	A-13
Chlorodifluoromethane (FREON-22)	CHClF <sub>2</sub>	86.469	96.154	A-13
Chlorodifluoromethane, Monodeuterated	CDClF <sub>2</sub>	87.475	95.048	A-14
Chloroform	CHCl <sub>3</sub>	119.378	69.647	A-14
Chlorofluoromethane	CH <sub>2</sub> ClF	68.478	121.415	A-14
Chloromethylidyne	CCl	47.464	175.171	A-15
Chlorosilane	SiH <sub>3</sub> Cl	66.563	124.909	A-15
Chlorotrifluoro- methane (FREON-13)	CClF <sub>3</sub>	104.459	79.594	A-15
Cumene	C <sub>6</sub> H <sub>5</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	120.196	69.173	A-15
Cyanogen	(CN) <sub>2</sub>	52.036	159.781	A-15
Cyanogen Chloride	CNCl	61.471	135.256	A-16
Cyclohexane - See Hexane				
Cyclopropane - See Propane				
n-Decane	C <sub>10</sub> H <sub>22</sub>	142.287	58.434	A-16
n-Deuterium	D <sub>2</sub>	4.028	2064.131	A-16
Deuterium (monatomic)	D	2.014	4128.262	A-17
Dibromomethane	CH <sub>2</sub> Br <sub>2</sub>	173.845	47.826	A-17
Dichlorodifluoro- methane (FREON-12)	CCl <sub>2</sub> F <sub>2</sub>	120.914	68.762	A-17
1,1-Dichloro-1- fluoroethane	CH <sub>3</sub> CFC1 <sub>2</sub>	116.951	71.093	A-17
Dichlorofluoromethane (FREON-21)	CHCl <sub>2</sub> F	102.924	80.782	A-17
Dichlorofluoromethane, Monodeuterated	CDCl <sub>2</sub> F	103.930	80.000	A-18
Dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	84.933	97.893	A-18
1,1-Dichlorotetra- fluoroethane	CCl <sub>2</sub> FCF <sub>3</sub>	170.922	48.644	A-18

TABLE A-I  
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Dichlorotetrafluoroethane (FREON-114)	$C_2Cl_2F_4$	170.922	48.644	A-18
2,2-Dichloro-1,1,1-trifluoroethane	$F_3CCHCl_2$	152.931	54.366	A-18
1,1-Difluoroethylene	$CH_2CF_2$	64.035	129.840	A-19
Difluoromethane	$CH_2F_2$	52.024	159.817	A-19
Dimethylamine	$(CH_3)_2NH$	45.085	184.415	A-19
2,2-Dimethylbutane	$CH_3CH_2C(CH_3)_3$	86.178	96.478	A-19
2,3-Dimethylbutane	$[(CH_3)_2CH]_2$	86.178	96.478	A-19
2,3-Dimethylhexane	$(CH_3)_2CHCH(CH_3)(CH_2)_2CH_3$	114.233	72.784	A-20
3,4-Dimethylhexane	$[CH(CH_3)CH_2CH_3]_2$	114.233	72.784	A-20
Dimethylpropane	$C(CH_3)_4$	72.151	115.234	A-20
Dipropylene Glycol	$(CH_3CHOHCH_2)_2O$	134.177	61.965	A-20
Dodecane	$CH_3(CH_2)_{10}CH_3$	170.341	48.810	A-20
Ethane	$C_2H_6$	30.070	276.498	A-21
Ethane, Hexadeuterated	$C_2D_6$	36.106	230.273	A-21
Ethanethiol	$C_2H_5SH$	62.134	133.812	A-21
Ethyl Acetate	$CH_3COOCH_2CH_3$	88.107	94.366	A-21
Ethyl Alcohol	$C_2H_5OH$	46.070	180.473	A-22
Ethylbenzene	$C_6H_5C_2H_5$	106.169	78.312	A-22
Ethyl Ether	$C_4H_{10}O$	74.124	112.168	A-22
Ethylene	$C_2H_4$	28.054	296.367	A-22
Ethylene Oxide	$(CH_2)_2O$	44.054	188.732	A-23
3-Ethylhexane	$(CH_3CH_2)_2CH(CH_2)_2CH_3$	114.233	72.784	A-23
3-Ethyl-2-methylpentane	$(CH_3)_2CHCH(C_2H_5)_2$	114.233	72.784	A-23
3-Ethyl-3-methylpentane	$(CH_3CH_2)_3CCH_3$	114.233	72.784	A-23
Fluorine	$F_2$	37.997	218.816	A-24
Fluorine (monatomic)	$F$	18.9984	437.633	A-24
Fluoroethane	$CH_3CH_2F$	48.061	172.997	A-24
Fluoroethylene	$CH_2CHF$	46.045	180.571	A-24
Fluoroform, Monodeut.	$CF_3D$	71.020	117.070	A-25
Fluoromethane	$CH_3F$	34.033	244.298	A-25
Formaldehyde	$HCHO$	30.026	276.899	A-25
Formyl	$HCO$	29.019	286.518	A-25
Furan	$C_4H_4O$	68.076	122.133	A-25
Helium	$He$	4.003	2077.022	A-26
n-Heptane	$C_7H_{16}$	100.206	82.973	A-26
Hexafluoroethane	$(CF_3)_2$	138.013	60.243	A-26
n-Hexane	$C_6H_{14}$	86.178	96.478	A-26

TABLE A-I  
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Cyclohexane	$C_6H_{12}$	84.163	98.789	A-27
Hydrazine	$N_2H_4$	32.045	259.455	A-27
Hydrobromic Acid	HBr	80.917	102.751	A-27
Hydrocyanic Acid	HCN	27.026	307.644	A-27
Hydrofluoric Acid	HF	20.006	415.584	A-28
Hydrofluoric Acid, Monodeuterated	DF	21.012	395.686	A-28
Hydrogen	$H_2$	2.016	4124.289	A-28
Hydrogen (Monatomic)	H	1.008	8248.579	A-29
Hydrogen, Monodeut.	HD	3.022	2751.291	A-29
Hydrogen Chloride	HCl	36.461	228.033	A-29
Hydrogen Iodide	HI	127.912	65.000	A-29
Hydrogen Peroxide	$H_2O_2$	34.015	244.433	A-29
Hydrogen Sulfide	$H_2S$	34.080	243.965	A-30
Hydrogen Sulfide, Dideuterated	$D_2S$	36.092	230.365	A-30
Hydrogen Sulfide, Ditritiated	$T_2S$	38.098	218.235	A-30
Hydrogen Sulfide, Monodeuterated	HDS	35.086	236.970	A-30
Hydrogen Sulfide, Monodeut/monotrit.	DTS	37.095	224.136	A-30
Hydrogen Sulfide, Monotritiated	HTS	36.089	230.384	A-31
Hydroxyl	OH	17.007	488.866	A-31
Iodine	$I_2$	253.809	32.758	A-31
Iodine (monatomic)	I	126.9044	65.516	A-31
Iodine Bromide	IBr	206.813	40.202	A-31
Iodine Chloride	ICl	162.357	51.210	A-31
Iodine Fluoride	IF	145.903	56.985	A-32
Iodine Heptafluoride	$IF_7$	259.893	31.991	A-32
Iodine Pentafluoride	$IF_5$	221.896	37.469	A-32
Iodomethane	$CH_3I$	141.939	58.577	A-32
Isoprene	$CH_2C(CH_3)CHCH_2$	68.120	122.055	A-32
Ketene	$H_2CCO$	42.038	197.783	A-33
Krypton	Kr	83.80	99.216	A-33
Mesitylene	$C_6H_3(CH_3)_3$	120.196	69.173	A-33
Methane	$CH_4$	16.043	518.251	A-33
Methane, Dideuterated	$CH_2D_2$	18.055	460.497	A-34
Methane, Dideut, Ditr. .	$CD_2T_2$	22.073	376.671	A-34
Methane, Ditr. .	$CH_2T_2$	20.061	414.450	A-34
Methane, Monodeut.	$CH_3D$	17.049	487.670	A-34

TABLE A-I  
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Methane, Monodeut., Tritritiated	$\text{CDT}_3$	23.076	360.299	A-34
Methane, Monotrit.	$\text{CH}_3\text{T}$	18.052	460.575	A-34
Methane, Tetradeut.	$\text{CD}_4$	20.067	414.325	A-35
Methane, Tetratrit.	$\text{CT}_4$	24.079	345.291	A-35
Methane, Trideut.	$\text{CHD}_3$	19.061	436.193	A-35
Methane, Trideut., Monotritiated	$\text{CD}_3\text{T}$	21.070	394.602	A-35
Methane, Tritritated	$\text{CHT}_3$	22.070	376.723	A-35
Methanethiol	$\text{CH}_3\text{SH}$	48.107	172.830	A-35
Methyl	$\text{CH}_3$	15.035	552.995	A-36
Methyl Acetate	$\text{CH}_3\text{COOCH}_3$	74.080	112.234	A-36
Methyl Alcohol	$\text{CH}_3\text{OH}$	32.042	259.478	A-36
Methylamine	$\text{CH}_3\text{NH}_2$	31.058	267.706	A-36
2-Methylbutane	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$	72.151	115.234	A-36
2-Methyl-2- butanol	$(\text{CH}_3)_2\text{COHCH}_2\text{CH}_3$	88.151	94.319	A-37
3-Methyl-1- butanol	$(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{OH}$	88.151	94.319	A-37
3-Methyl-1-butyne	$(\text{CH}_3)_2\text{CHCCH}$	68.120	122.055	A-37
Methyl Chloride	$\text{CH}_3\text{Cl}$	50.488	164.679	A-37
Methyl Cyanide	$\text{CH}_3\text{CN}$	41.053	202.527	A-38
Methyl Ether	$(\text{CH}_3)_2\text{O}$	46.070	180.473	A-38
Methylhydrazine	$\text{CH}_3\text{NHNH}_2$	46.072	180.462	A-38
Methylidyne	$\text{CH}$	13.019	638.624	A-38
Methyl Isocyanide	$\text{CH}_3\text{NC}$	41.053	202.527	A-38
2-Methylpentane	$(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{CH}_3$	86.178	96.478	A-39
3-Methylpentane	$[\text{CH}_2\text{CH}_2]_2\text{CH}(\text{CH}_3)$	86.178	96.478	A-39
4-Methyl-2- pentanone	$\text{CH}_3\text{COCH}_2\text{CH}(\text{CH}_3)_2$	100.162	83.009	A-39
2-Methyl-1- propanol	$(\text{CH}_3)_2\text{CHCH}_2\text{OH}$	74.124	112.168	A-39
2-Methyl-2-propanol	$(\text{CH}_3)_3\text{COH}$	74.124	112.168	A-40
2-Methylpropene	$(\text{CH}_3)_2\text{CCH}_2$	56.108	148.183	A-40
Methyl Sulfide	$(\text{CH}_3)_2\text{S}$	62.134	133.812	A-40
Neon	$\text{Ne}$	20.183	411.947	A-40
Nitric Oxide	$\text{NO}$	30.006	277.088	A-40
Nitrogen	$\text{N}_2$	28.013	296.798	A-41
Nitrogen (Monatomic)	$\text{N}$	14.0067	593.596	A-41
Nitrous Oxide	$\text{N}_2\text{O}$	44.013	188.907	A-41
n-Nonane	$\text{C}_9\text{H}_{20}$	128.260	64.824	A-42
n-Octane	$\text{C}_8\text{H}_{18}$	114.233	72.784	A-42

TABLE A-I  
(CONT.)

NAME	FORMULA	AT.WT/ MOL WT	GAS CONST	APP A PAGE
Oxygen	O <sub>2</sub>	31.999	259.832	A-42
Oxygen (Monatomic)	O	15.9994	519.664	A-43
Oxygen Fluoride	OF <sub>2</sub>	53.996	153.980	A-43
n-Pentane	C <sub>5</sub> H <sub>12</sub>	72.151	115.234	A-44
1-Pentanol	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> OH	88.151	94.319	A-44
3-Pentanone	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	86.135	96.527	A-44
1-Pentene	CH <sub>2</sub> CH(CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	70.135	118.547	A-45
1-Pentyne	HCCCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	68.120	122.055	A-45
2-Pentyne	CH <sub>3</sub> CCCH <sub>2</sub> CH <sub>3</sub>	68.120	122.055	A-45
Phosgene	COCl <sub>2</sub>	98.917	84.054	A-45
Phosphine	PH <sub>3</sub>	33.998	244.555	A-46
Phosphine, Trideut. PD <sub>3</sub>	PD <sub>3</sub>	37.016	224.615	A-46
Phosphorus Trichloride	PCl <sub>3</sub>	137.333	60.541	A-46
Phosphorus Trifluoride	PF <sub>3</sub>	87.969	94.514	A-46
Propadiene	C(CH <sub>2</sub> ) <sub>2</sub>	40.065	207.519	A-46
Propane	C <sub>3</sub> H <sub>8</sub>	44.097	188.545	A-47
Cyclopropane	C <sub>3</sub> H <sub>6</sub>	44.097	188.545	A-47
1,2-Propanediol	CH <sub>3</sub> CHOHCH <sub>2</sub> OH	76.096	109.261	A-47
1-Propanol	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> OH	60.097	138.349	A-47
2-Propanol	(CH <sub>3</sub> ) <sub>2</sub> CHOH	60.097	138.349	A-48
Propylbenzene	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	120.196	69.173	A-48
Propyl Ether	[CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> O	102.178	81.371	A-48
Propyne	CH <sub>3</sub> CCH	40.065	207.519	A-48
Silane	SiH <sub>4</sub>	32.118	258.869	A-49
Silicon Tetrachloride	SiCl <sub>4</sub>	169.898	48.937	A-49
Silicon Tetrafluoride	SiF <sub>4</sub>	104.080	79.884	A-49
Styrene	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	104.153	79.828	A-49
Sulfur	S <sub>2</sub>	64.128	129.652	A-49
Sulfur (monatomic)	S	32.064	259.304	A-49
Sulfur Dichloride	SCl <sub>2</sub>	102.970	80.745	A-50
Sulfur Difluoride	SF <sub>2</sub>	70.061	118.673	A-50
Sulfur Dioxide	SO <sub>2</sub>	64.063	129.784	A-50
Sulfur Hexafluoride	SF <sub>6</sub>	146.054	56.926	A-50
Sulfur Monochloride	S <sub>2</sub> Cl <sub>2</sub>	135.034	61.572	A-50
Sulfur Monoxide	SO	48.063	172.987	A-50
Sulfur Tetrafluoride	SF <sub>4</sub>	108.058	76.943	A-51
Sulfur Trioxide	SO <sub>3</sub>	80.062	103.848	A-51
Sulfuryl Fluoride	SO <sub>2</sub> F <sub>2</sub>	102.060	81.465	A-51
Thionyl Chloride	SOCl <sub>2</sub>	118.969	69.886	A-51
Thionyl Fluoride	SOF <sub>2</sub>	86.060	96.611	A-51
Thiophosgene	CSCl <sub>2</sub>	114.981	72.310	A-51
Toluene	C <sub>7</sub> H <sub>8</sub>	92.142	90.234	A-52
1,1,1-Trichloroethane	CH <sub>3</sub> CCl <sub>3</sub>	133.405	62.324	A-52

TABLE A-I  
(CONT.)

NAME	FORMULA	AT WT/ MOL WT	GAS CONST	APP A PAGE
Trichlorofluoro- methane (FREON-11)	$\text{CCl}_3\text{F}$	137.369	60.526	A-52
Trichlorotrifluoro- ethane (FREON-113)	$\text{C}_2\text{Cl}_3\text{F}_3$	187.377	44.372	A-53
Trichlorosilane	$\text{SiHCl}_3$	135.453	61.382	A-53
1,1,1-trichloro-2,2,2- trifluoroethane	$\text{CF}_3\text{CCl}_3$	187.377	44.372	A-53
1,1,1-Trifluoroethane	$\text{CH}_3\text{CF}_3$	84.041	98.931	A-53
Trifluoroiodomethane	$\text{CF}_3\text{I}$	195.911	42.439	A-54
Trimethylamine	$(\text{CH}_3)_3\text{N}$	59.112	140.654	A-54
2,3,4-Trimethyl-[(CH <sub>3</sub> ) <sub>2</sub> CH] <sub>2</sub> CHCH <sub>3</sub> pentane		114.233	72.784	A-54
Water	$\text{H}_2\text{O}$	18.015	461.513	A-54
Water, Dideuterated	$\text{D}_2\text{O}$	20.027	415.147	A-55
Xenon	$\text{Xe}$	131.30	63.323	A-55
m-Xylene	$\text{C}_6\text{H}_4(\text{CH}_3)_2$	106.169	78.312	A-55
o-Xylene	$\text{C}_6\text{H}_4(\text{CH}_3)_2$	106.169	78.312	A-56
p-Xylene	$\text{C}_6\text{H}_4(\text{CH}_3)_2$	106.169	78.312	A-56

# APPENDIX A FORMAT EXAMPLE

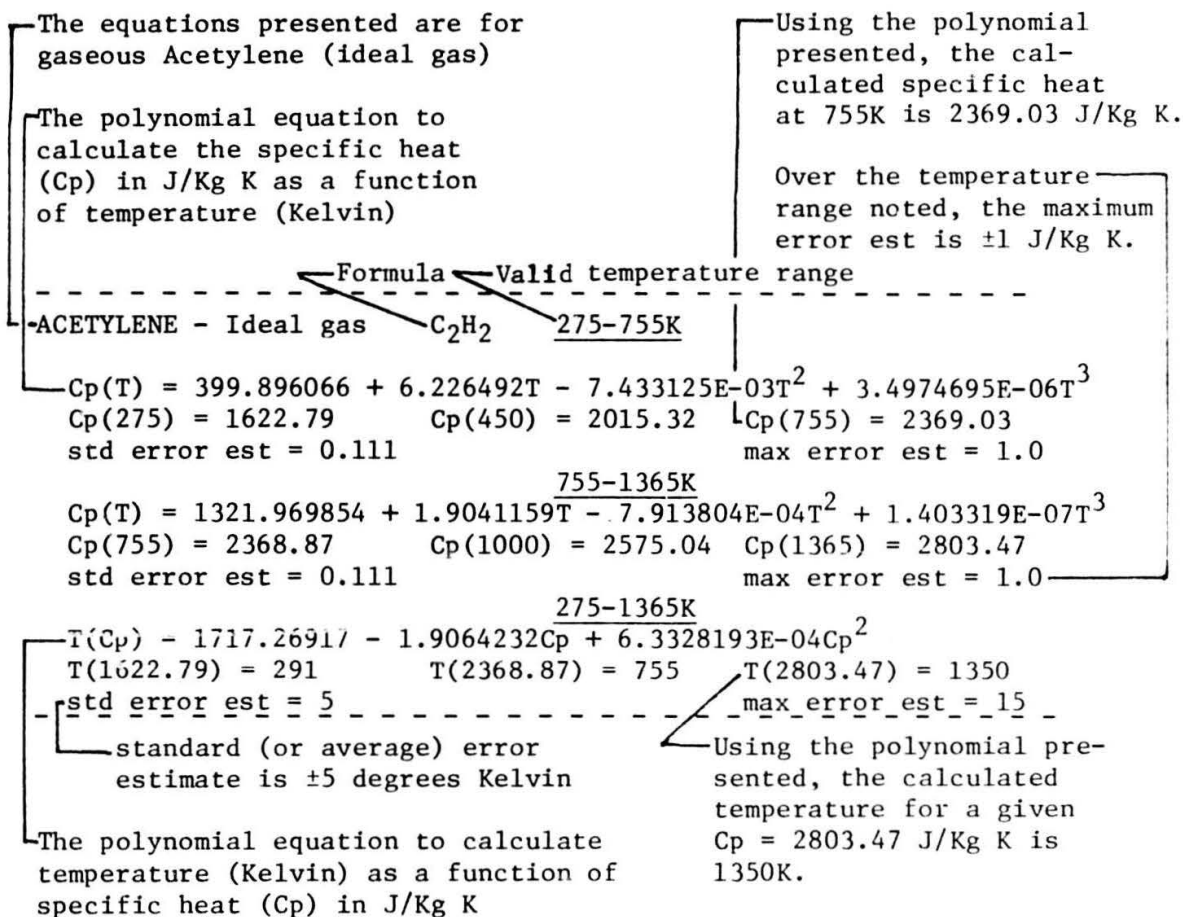


FIGURE A-1

# APPENDIX A

## SPECIFIC HEAT AT CONSTANT PRESSURE FOR GASEOUS ELEMENTS AND COMPOUNDS

-----  
ACETONE - Ideal gas  $C_3H_6O$  275-1365K

$$C_p(T) = 345.6240845 + 3.1344046T + 9.000608E-04T^2 - 1.9981015E-06T^3 \\ - 7.2481823E-10T^4 + 1.757756E-12T^5 - 5.94192596E-16T^6$$

$$C_p(275) = 1232.46 \quad C_p(700) = 2346.88 \quad C_p(1365) = 3189.13 \\ \text{std error est} = 0.791 \quad \text{max error est} = 1.25$$

275-1365K

$$T(C_p) = -537.70187 + 1.08064298C_p - 4.673706E-04C_p^2 + 9.857246E-08C_p^3$$

$$T(1232.46) = 269 \quad T(2346.88) = 698 \quad T(3189.13) = 1352$$

std error est = 3 ----- max error est = 13 -----

ACETYLENE - Ideal gas  $C_2H_2$  275-755K

$$C_p(T) = 399.896066 + 6.226492T - 7.433125E-03T^2 + 3.4974695E-06T^3$$

$$C_p(275) = 1622.79 \quad C_p(450) = 2015.32 \quad C_p(755) = 2369.03 \\ \text{std error est} = 0.111 \quad \text{max error est} = 1.0$$

755-1365K

$$C_p(T) = 1321.969854 + 1.9041159T - 7.913804E-04T^2 + 1.403319E-07T^3$$

$$C_p(755) = 2368.87 \quad C_p(1000) = 2575.04 \quad C_p(1365) = 2803.47 \\ \text{std error est} = 0.111 \quad \text{max error est} = 1.0$$

275-1365K

$$T(C_p) = 1717.26917 - 1.9064232C_p + 6.3328193E-04C_p^2$$

$$T(1622.79) = 291 \quad T(2368.87) = 755 \quad T(2803.47) = 1350$$

std error est = 5 ----- max error est = 15 -----

AIR - Ideal gas 100-590K

$$C_p(T) = 1022.5294853 - 0.1758625T + 4.020605E-04T^2 - 4.8640623E-08T^3$$

$$C_p(100) = 1008.92 \quad C_p(350) = 1008.14 \quad C_p(590) = 1048.74 \\ \text{std error est} = 0.012 \quad \text{max error est} = 0.025$$

590-1365K

$$C_p(T) = 928.911894 + 0.0897769T + 3.2460657E-04T^2 - 2.62542E-07T^3$$

$$+ 5.99901E-11T^4 \\ C_p(590) = 1048.22 \quad C_p(1000) = 1140.74 \quad C_p(1365) = 1196.81 \\ \text{std error est} = 0.22 \quad \text{max error est} = 0.5$$

590-1365K

$$T(C_p) = -100444.9907 + 275.16644C_p - 0.253212C_p^2 + 7.885293E-05C_p^3$$

$$T(1048.22) = 588 \quad T(1140.74) = 998 \quad T(1196.81) = 1361$$

$$\text{std error est} = 1.5 \quad \text{max error est} = 4$$

Note: For  $T(C_p)$  calculations below 590K use the iterative procedures discussed in Section 5 and the following polynomial: 100-590K,

$$C_p(T) = 1021.17215 - 0.1603904T + 3.5182525E-04T^2.$$



AIR - Real gas

255-865K

$$Cp(T) = 1052.71406 - 0.3745355T + 8.361477E-04T^2 - 3.32111E-07T^3 \\ - 4.683905E-11T^4$$

$$Cp(255) = 1005.87 \quad Cp(560) = 1042.26 \quad Cp(865) = 1113.2 \\ \text{std error est} = 0.17 \quad \text{max error est} = 0.4$$

Note: For T(Cp) calculations use the iterative procedures discussed in Section 5 and the following polynomial: 255-865K, Cp(T) =

$$-996.831581 - 0.0322256T + 2.0181265E-04T^2 \quad \text{-----}$$

AMMONIA - Ideal gas NH<sub>3</sub> 220-590K

$$Cp(T) = 1948.475605 - 0.81912827T + 5.424779E-03T^2 - 3.60715E-06T^3 \\ Cp(220) = 1992.42 \quad Cp(400) = 2257.93 \quad Cp(590) = 2612.72 \\ \text{std error est} = 0.12 \quad \text{max error est} = 1.0$$

590-1365K

$$Cp(T) = 2124.419956 - 1.746889T + 8.22758E-03T^2 - 8.855634E-06T^3 \\ + 4.420294E-09T^4 - 8.734964E-13T^5 \\ Cp(590) = 2612.19 \quad Cp(1000) = 3296.27 \quad Cp(1365) = 3753.45 \\ \text{std error est} = 0.36 \quad \text{max error est} = 1.0$$

220-590K

$$T(Cp) = -8836.6068 + 10.54741Cp - 4.154804E-03Cp^2 + 5.737145E-07Cp^3 \\ T(1992.42) = 222 \quad T(2257.93) = 401 \quad T(2612.72) = 591 \\ \text{std error est} = 0.8 \quad \text{max error est} = 2.0$$

590-1365K

$$T(Cp) = -2501.9985 + 2.45231Cp - 7.299265E-04Cp^2 + 9.350415E-08Cp^3 \\ T(2612.19) = 590 \quad T(3296.27) = 999 \quad T(3753.45) = 1364 \\ \text{std error est} = 0.5 \quad \text{max error est} = 2.0$$

ARGON - Ideal gas Ar 0-6000K

$$Cp = 520.34 \text{ (constant)} \quad \text{-----}$$

ARSINE AsH<sub>3</sub> 300-1000K

$$Cp(T) = 347.13902 + 0.231073T + 1.309066E-03T^2 - 1.577571E-06T^3 \\ + 5.450638E-10T^4 \\ Cp(300) = 496.1 \quad Cp(600) = 686.93 \quad Cp(1000) = 854.77 \\ \text{std error est} = 1.13 \quad \text{max error est} = 2.0$$

300-1000K

$$T(Cp) = -1935.0966 + 9.24965Cp - 1.33801E-02Cp^2 + 7.69057E-06Cp^3 \\ T(496.1) = 300 \quad T(686.93) = 598 \quad T(854.77) = 998 \\ \text{std error est} = 3.3 \quad \text{max error est} = 5.0$$

ARSINE, Trideuterated AsD<sub>3</sub> 300-1000K

$$Cp(T) = 245.545853 + 1.09726T - 3.84163E-05T^2 - 8.056253E-07T^3 \\ + 4.042793E-10T^4 \\ Cp(300) = 552.79 \quad Cp(600) = 768.45 \quad Cp(1000) = 903.04$$

ARSINE, Trideuterated (continued)

std error est = 0.43

max error est = 2.0

$$T(Cp) = 8581.361485 - 52.568517Cp + 0.121435Cp^2 - 1.22502E-04Cp^3 + 4.6727183E-08Cp^4$$

$$T(552.79) = 300 \quad T(768.45) = 599 \quad T(903.04) = 1000$$

$$\text{std error est} = 1.3 \quad \text{max error est} = 3.0$$

BENZENE - Ideal gas  $C_6H_6$  275-1365K

$$Cp(T) = -297.4345373 + 4.42278708T + 2.810036E-03T^2 - 1.136955E-05T^3 + 1.1190287E-08T^4 - 4.8717996E-12T^5 + 8.019155E-16T^6$$

$$Cp(275) = 951.57 \quad Cp(800) = 2415.38 \quad Cp(1365) = 3008.37$$

$$\text{std error est} = 0.67 \quad \text{max error est} = 1.3$$

$$T(Cp) = 392.0602 - 0.648326Cp + 8.326166E-04Cp^2 - 3.4749E-07Cp^3 + 5.9114275E-11Cp^4$$

$$T(951.57) = 278 \quad T(2415.38) = 799 \quad T(3008.37) = 1358$$

$$\text{std error est} = 1.6 \quad \text{max error est} = 7$$

BENZENE - Real gas 300-600K

$$Cp(T) = -283.22595 + 5.300935T - 2.4209348E-03T^2$$

$$Cp(300) = 1089.17 \quad Cp(450) = 1611.96 \quad Cp(600) = 2025.8$$

$$\text{std error est} = 0.9 \quad \text{max error est} = 1.5$$

$$T(Cp) = 129.444998 + 0.07207415Cp + 7.8699477E-05Cp^2$$

$$T(1089.17) = 301 \quad T(1611.96) = 450 \quad T(2025.8) = 598$$

BORON FLUORIDE OXIDE, (BOF)<sub>3</sub> 300-500K

Trimeric

$$Cp(T) = 79.2504 + 3.2856459T - 2.3282776E-03T^2$$

$$Cp(300) = 855.4 \quad Cp(400) = 1021 \quad Cp(500) = 1140$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 1.0$$

$$T(Cp) = 505.381375 - 0.9481142Cp + 8.275349E-04Cp^2$$

$$T(855.4) = 300 \quad T(1021) = 400 \quad T(1140) = 500$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.0$$

BORON TRIBROMIDE  $BBr_3$  300-1000K

$$Cp(T) = 140.1554722 + 0.71322266T - 1.1636584E-03T^2 + 9.112207E-07T^3 - 2.780408E-10T^4$$

$$Cp(300) = 271.74 \quad Cp(650) = 312.72 \quad Cp(1000) = 322.9$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.0$$

Note: For T(Cp) calculations use the iterative procedures discussed in Section 5 and:  $Cp(T) = 212.708133 + 0.24356T - 1.35451E-04T^2$

BORON TRICHLORIDE  $\text{BCl}_3$ 100-1500K

$$\text{Cp}(T) = 188.655802 + 1.888567T - 3.184433E-03T^2 + 2.8712E-06T^3 - 1.3291673E-09T^4 + 2.474797E-13T^5$$

$$\text{Cp}(100) = 348.8 \quad \text{Cp}(800) = 668.19 \quad \text{Cp}(1500) = 697.22$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1.0$$

BORON TRIFLUORIDE  $\text{BF}_3$ 145-645K

Ideal gas

$$\text{Cp}(T) = 298.65561 + 1.865263T - 1.3085604E-03T^2 + 1.995E-07T^3$$

$$\text{Cp}(145) = 542.21 \quad \text{Cp}(400) = 848.16 \quad \text{Cp}(645) = 1010.89$$

$$\text{std error est} = 0.24 \quad \text{max error est} = 1.0$$

645-1365K

$$\text{Cp}(T) = 466.430362 + 1.331415T - 8.914198E-04T^2 + 2.12377E-07T^3$$

$$\text{Cp}(645) = 1011.33 \quad \text{Cp}(1000) = 1118.80 \quad \text{Cp}(1365) = 1163.04$$

$$\text{std error est} = 0.11 \quad \text{max error est} = 1.0$$

145-645K

$$T(\text{Cp}) = 1438.87308 - 8.75606\text{Cp} + 0.020047\text{Cp}^2 - 1.908134E-05\text{Cp}^3$$

$$+ 6.971855E-09\text{Cp}^4$$

$$T(542.21) = 146 \quad T(848.16) = 399 \quad T(1010.89) = 642$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 3.0$$

645-1365K

$$T(\text{Cp}) = -180147.73 + 519.93406\text{Cp} - 0.5005\text{Cp}^2 + 1.613357E-04\text{Cp}^3$$

$$T(1011.33) = 653 \quad T(1118.80) = 1009 \quad T(1163.04) = 1362$$

$$\text{std error est} = 5.2 \quad \text{max error est} = 12$$

BROMINE - Ideal gas  $\text{Br}_2$ 200-590K

$$\text{Cp}(T) = 175.261725 + 0.304817T - 5.66955E-04T^2 + 3.5797E-07T^3 + 1.30779E-11T^4$$

$$\text{Cp}(200) = 216.43 \quad \text{Cp}(400) = 229.72 \quad \text{Cp}(590) = 232.85$$

$$\text{std error est} = 1.2E-02 \quad \text{max error est} = 0.2$$

590-1365K

$$\text{Cp}(T) = 223.7002 + 2.231436E-02T - 1.335276E-05T^2 + 3.0736E-09T^3$$

$$\text{Cp}(590) = 232.85 \quad \text{Cp}(1000) = 235.74 \quad \text{Cp}(1365) = 237.097$$

$$\text{std error est} = 9.9E-03 \quad \text{max error est} = 0.2$$

200-590K

$$T(\text{Cp}) = -649483.9088 + 2282.92562\text{Cp} + 48.1995412\text{Cp}^2 - 0.335799\text{Cp}^3$$

$$+ 5.93457E-04\text{Cp}^4$$

$$T(216.43) = 183 \quad T(229.72) = 402 \quad T(232.85) = 589$$

$$\text{std error est} = 6.0 \quad \text{max error est} = 17.0$$

590-1365K

$$T(\text{Cp}) = 1327415.6666 - 11467.00468\text{Cp} + 24.77498\text{Cp}^2$$

$$T(232.85) = 601 \quad T(235.74) = 1013 \quad T(237.097) = 1348$$

$$\text{std error est} = 7.0 \quad \text{max error est} = 21$$

BROMINE (Monatomic) B 250-1500K

$C_p(T) = 264.48344899 - 2.672822E-02T + 4.013018E-05T^2 - 1.04915E-08T^3$   
 $C_p(250) = 260.14$   $C_p(900) = 265.29$   $C_p(1500) = 279.28$   
 std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed  
 in Section 5 and the following eqn: 250-1500K,  $C_p(T) = 260.01432$   
 $- 5.58942E-03T + 1.263795E-05T^2$ .

BROMINE CHLORIDE BrCl 250-1500K

$C_p(T) = 194.97556 + 0.764857T - 2.058934E-03T^2 + 3.0416852E-06T^3$   
 $- 2.5048785E-09T^4 + 1.07526E-12T^5 - 1.870628E-16T^6$   
 $C_p(250) = 296.25$   $C_p(900) = 325.06$   $C_p(1500) = 328.89$   
 std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed  
 in Section 5 and the following eqn: 250-1500K,  $C_p(T) = 283.400876$   
 $+ 7.585277E-02T - 3.15832E-05T^2$ .

BROMINE FLUORIDE BrF 250-1500K

$C_p(T) = 241.432653 + 0.456866T - 6.069283E-04T^2 + 3.694047E-07T^3$   
 $- 8.374216E-11T^4$   
 $C_p(250) = 323.16$   $C_p(900) = 375.35$   $C_p(1500) = 383.94$   
 std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed  
 in Section 5 and the following eqn: 250-1500K,  $C_p(T) = 266.492708$   
 $+ 0.291667T - 2.572893E-04T^2 + 7.705475E-08T^3$ .

BROMINE PENTAFLUORIDE BrF<sub>5</sub> 250-1500K

$C_p(T) = -106.97977 + 4.406352T - 1.040336E-02T^2 + 1.362716E-05T^3$   
 $- 1.013227E-08T^4 + 3.9961242E-12T^5 - 6.484931E-16T^6$   
 $C_p(250) = 521.49$   $C_p(900) = 733.47$   $C_p(1500) = 750.86$   
 std error est = 0.51 max error est = 1.0

BROMOFORM CHBr<sub>3</sub> 100-1500K

$C_p(T) = 142.57457 + 0.651772857T - 5.93501E-04T^2 + 1.831537E-07T^3$   
 $C_p(100) = 202.0$   $C_p(900) = 381.95$   $C_p(1500) = 403.0$   
 std error est = 0.01 max error est = 0.1

Note: For T(Cp) calculations, use the iterative procedures discussed  
 in Section 5 and the equation above.

BROMOMETHANE  $\text{CH}_3\text{Br}$  300-1200K

$\text{Cp}(T) = 145.940214 + 1.19246T - 6.440412\text{E-}04T^2 + 1.4439654\text{E-}07T^3$   
 $\text{Cp}(300) = 449.61$   $\text{Cp}(800) = 761.65$   $\text{Cp}(1200) = 898.99$   
std error est = 1.33 max error est = 3.0

300-1200K

$T(\text{Cp}) = -799.119 + 4.44998\text{Cp} - 6.457116\text{E-}03\text{Cp}^2 + 4.4251195\text{E-}06\text{Cp}^3$   
 $T(449.61) = 298$   $T(761.65) = 800$   $T(898.99) = 1198$   
- std error est = 2.6 - - - - - max error est = 5.0 -

BROMOTRICHLORO-  $\text{CCl}_3\text{Br}$  100-1500K  
METHANE

$\text{Cp}(T) = 113.19427 + 1.6936076T - 2.71334\text{E-}03T^2 + 1.949586\text{E-}06T^3$   
-  $5.11705\text{E-}10T^4$   
 $\text{Cp}(100) = 257.32$   $\text{Cp}(900) = 525.15$   $\text{Cp}(1500) = 537.94$   
- std error est = 3.2 - - - - - max error est = 6.0 -

1,3-BUTADIENE  $(\text{CH}_2\text{CH})_2$  275-1500K

$\text{Cp}(T) = -254.813554 + 7.020756T - 3.20957\text{E-}03T^2 - 5.334136\text{E-}06T^3$   
+  $8.92008\text{E-}09T^4 - 5.015366\text{E-}12T^5 + 1.006158\text{E-}15T^6$   
 $\text{Cp}(275) = 1365.8$   $\text{Cp}(900) = 3001.2$   $\text{Cp}(1500) = 3585.32$   
std error est = 1.33 max error est = 6.0

275-1500K

$T(\text{Cp}) = 857.73873 - 1.465754\text{Cp} + 1.1834\text{E-}03\text{Cp}^2 - 3.7378\text{E-}07\text{Cp}^3$   
+  $4.785293\text{E-}11\text{Cp}^4$   
 $T(1365.8) = 278$   $T(3001.2) = 896$   $T(3585.32) = 1495$   
- std error est = 3.5 - - - - - max error est = 5.0 -

iso-BUTANE  $\text{i-C}_4\text{H}_{10}$  275-1365K  
Ideal gas

$\text{Cp}(T) = -78.01978396 + 6.892987T - 4.385152\text{E-}03T^2 + 4.553157\text{E-}06T^3$   
-  $6.538463\text{E-}09T^4 + 4.658174\text{E-}12T^5 - 1.18572476\text{E-}15T^6$   
 $\text{Cp}(275) = 1550.03$   $\text{Cp}(900) = 3723.52$   $\text{Cp}(1365) = 4445.63$   
std error est = 1.05 max error est = 2.1

275-1365K

$T(\text{Cp}) = 232.4366 - 0.244747\text{Cp} + 2.728018\text{E-}04\text{Cp}^2 - 7.6475562\text{E-}08\text{Cp}^3$   
+  $9.0742275\text{E-}12\text{Cp}^4$   
 $T(1550.03) = 276$   $T(3723.52) = 900$   $T(4445.63) = 1361$   
std error est = 1.0 max error est = 4.0

iso-BUTANE - Real gas 275-710K

$\text{Cp}(T) = 1700.20484 - 16.818853T + 0.1295973T^2 - 3.956676\text{E-}04T^3$   
+  $6.527002\text{E-}07T^4 - 5.60803\text{E-}10T^5 + 1.96009\text{E-}13T^6$   
 $\text{Cp}(275) = 1582.82$   $\text{Cp}(500) = 2562.96$   $T(710) = 3264.21$   
std error est = 1.2 max error est = 1.8

275-710K

$T(\text{Cp}) = 82.72775 + 0.05989134\text{Cp} + 4.0183998\text{E-}05\text{Cp}^2$   
 $T(1582.82) = 278$   $T(2562.96) = 500$   $T(3264.21) = 706$

iso-BUTANE - Real gas (continued)

std error est = 1.7 max error est = 6

n-BUTANE  $\text{n-C}_4\text{H}_{10}$  265-755K

Ideal gas

$$\text{Cp}(T) = 236.65134 + 5.10573T - 4.16089E-04T^2 - 1.1450804E-06T^3$$

$$\text{Cp}(265) = 1539.14 \quad \text{Cp}(500) = 2542.36 \quad \text{Cp}(755) = 3361.49$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.0$$

755-1365K

$$\text{Cp}(T) = 4401.26486 - 13.90866545T + 3.471109E-02T^2 - 3.45278E-05T^3$$

$$+ 1.619382E-08T^4 - 2.966666E-12T^5$$

$$\text{Cp}(755) = 3360.77 \quad \text{Cp}(1000) = 3903.04 \quad \text{Cp}(1365) = 4436.19$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 1.5$$

265-1365K

$$T(\text{Cp}) = -372.95792 + 0.63692878\text{Cp} - 1.95552E-04\text{Cp}^2 + 3.149068E-08\text{Cp}^3$$

$$T(3360.77) = 754 \quad T(3903.04) = 1006 \quad T(4436.19) = 1353$$

std error est = 3.5 max error est = 12

1-BUTANOL  $\text{CH}_3(\text{CH}_2)_3\text{OH}$  395-605K

$$\text{Cp}(T) = 740069.2476 - 7408.748863T + 29.59687066T^2 - 5.88465E-02T^3$$

$$+ 5.82563958E-05T^4 - 2.297227E-08T^5$$

$$\text{Cp}(395) = 2048.05 \quad \text{Cp}(500) = 2241.28 \quad \text{Cp}(605) = 2555.35$$

$$\text{std error est} = 16.0 \quad \text{max error est} = 23.0$$

Note: This is an extremely poor fit of the tabular data. The max

error est of 23 represents an error of 1.2% of the table data.

2-BUTANONE  $\text{CH}_3\text{CH}_2\text{COCH}_3$  275-1275K

$$\text{Cp}(T) = 20.545066 + 7.021058T - 1.15892E-02T^2 + 1.631369E-05T^3$$

$$- 1.31136E-08T^4 + 4.917275E-12T^5 - 5.9919712E-16T^6$$

$$\text{Cp}(275) = 1346.65 \quad \text{Cp}(800) = 2655.8 \quad \text{Cp}(1275) = 3284.96$$

std error est = 6.6 max error est = 12 (0.9%)

1-BUTENE  $\text{CH}_2\text{CHCH}_2\text{CH}_3$  275-1500K

$$\text{Cp}(T) = 139.59317 + 4.97386775T + 1.700397E-03T^2 - 9.414594E-06T^3$$

$$+ 1.0035756E-08T^4 - 4.7956263E-12T^5 + 8.828364E-16T^6$$

$$\text{Cp}(275) = 1490.44 \quad \text{Cp}(900) = 3352.02 \quad \text{Cp}(1500) = 4097.32$$

$$\text{std error est} = 1.12 \quad \text{max error est} = 2.5$$

275-1500K

$$T(\text{Cp}) = 739.649 - 1.1519803\text{Cp} + 8.633103E-04\text{Cp}^2 - 2.397716E-07\text{Cp}^3$$

$$+ 2.6524417E-11\text{Cp}^4$$

$$T(1490.44) = 277 \quad T(3352.02) = 896 \quad T(4097.32) = 1496$$

std error est = 3.2 max error est = 6.0

2-BUTENE (CH<sub>3</sub>CH)<sub>2</sub> 300-1000K

$$\begin{aligned} \text{Cp}(T) &= -53.440476 + 5.5916666T - 2.05714285E-03T^2 \\ \text{Cp}(300) &= 1438.92 \quad \text{Cp}(600) = 2560.99 \quad \text{Cp}(1000) = 3481.08 \\ \text{std error est} &= 0.23 \quad \text{max error est} = 1.0 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) &= 470.8465 - 0.72122159\text{Cp} + 6.591403E-04\text{Cp}^2 - 2.020906E-07\text{Cp}^3 \\ &\quad + 2.435593E-11\text{Cp}^4 \\ T(1438.92) &= 300 \quad T(2560.99) = 600 \quad T(3481.08) = 999 \\ \text{std error est} &= 1.4 \quad \text{max error est} = 3 \end{aligned}$$

cis-2-BUTENE (CH<sub>3</sub>CH)<sub>2</sub> 275-1500K

$$\begin{aligned} \text{Cp}(T) &= 593.119884 - 0.25533449T + 1.75336E-02T^2 - 3.26788E-05T^3 \\ &\quad + 2.844997E-08T^4 - 1.2341584E-11T^5 + 2.139958E-15T^6 \\ \text{Cp}(275) &= 1313.49 \quad \text{Cp}(900) = 3258.39 \quad \text{Cp}(1500) = 4054.29 \\ \text{std error est} &= 1.3 \quad \text{max error est} = 3.0 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) &= 367.106 - 0.531809\text{Cp} + 5.3353694E-04\text{Cp}^2 - 1.6407E-07\text{Cp}^3 \\ &\quad + 2.0168237E-11\text{Cp}^4 \\ T(1313.49) &= 277 \quad T(3258.39) = 896 \quad T(4054.29) = 1496 \\ \text{std error est} &= 3.5 \quad \text{max error est} = 5.0 \end{aligned}$$

trans-2-BUTENE (CH<sub>3</sub>CH)<sub>2</sub> 275-1500K

$$\begin{aligned} \text{Cp}(T) &= 725.45579 + 0.662269T + 1.2774909E-02T^2 - 2.40152E-05T^3 \\ &\quad + 2.06644E-08T^4 - 8.859714E-12T^5 + 1.5207345E-15T^6 \\ \text{Cp}(275) &= 1479.15 \quad \text{Cp}(900) = 3296.61 \quad \text{Cp}(1500) = 4068.29 \\ \text{std error est} &= 1.2 \quad \text{max error est} = 3.5 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) &= 525.129 - 0.865304\text{Cp} + 7.3369042E-04\text{Cp}^2 - 2.134057E-07\text{Cp}^3 \\ &\quad + 2.4521456E-11\text{Cp}^4 \\ T(1479.15) &= 277 \quad T(3296.61) = 897 \quad T(4068.29) = 1496 \\ \text{std error est} &= 3 \quad \text{max error est} = 5 \end{aligned}$$

BUTYL ETHER [CH<sub>3</sub>(CH<sub>2</sub>)<sub>3</sub>]<sub>2</sub>O 275-1275K

$$\begin{aligned} \text{Cp}(T) &= 2220.96497 - 15.85878T + 8.3621339E-02T^2 - 1.752393E-04T^3 \\ &\quad + 1.899729E-07T^4 - 1.0442973E-10T^5 + 2.2914465E-14T^6 \\ \text{Cp}(275) &= 1471.38 \quad \text{Cp}(800) = 2929.33 \quad \text{Cp}(1275) = 3333.16 \\ \text{std error est} &= 9.0 \quad \text{max error est} = 15.0 \end{aligned}$$

1-BUTYNE CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> 300-1500K

$$\begin{aligned} \text{Cp}(T) &= 138.2438 + 5.66515T - 4.1092457E-03T^2 + 1.692264E-06T^3 \\ &\quad - 3.051742E-10T^4 \\ \text{Cp}(300) &= 1511.18 \quad \text{Cp}(800) = 2781.89 \quad \text{Cp}(1500) = 3556.61 \\ \text{std error est} &= 0.95 \quad \text{max error est} = 2.0 \end{aligned}$$

1-BUTYNE (continued) 300-1500K  
 $T(Cp) = 1283.405 - 2.300184Cp + 1.743335E-03Cp^2 - 5.255778E-07Cp^3$   
 $+ 6.240944E-11Cp^4$   
 $T(1511.18) = 300 \quad T(2781.89) = 799 \quad T(3556.61) = 1496$   
 $\text{std error est} = 2.9 \quad \text{max error est} = 5.0$

2-BUTYNE  $(CH_3C)_2$  275-1500K  
 $Cp(T) = 724.78375 + 0.9002168T + 8.83253E-03T^2 - 1.6193317E-05T^3$   
 $+ 1.3383997E-08T^4 - 5.528233E-12T^5 + 9.190746E-16T^6$   
 $Cp(275) = 1371.78 \quad Cp(800) = 2718.32 \quad Cp(1500) = 3541.16$   
 $\text{std error est} = 2.3 \quad \text{max error est} = 3.5$   
275-1500K  
 $T(Cp) = 654.8792 - 1.297667Cp + 1.18347475E-03Cp^2 - 3.8756E-07Cp^3$   
 $+ 4.963734E-11Cp^4$   
 $T(1371.78) = 277 \quad T(2718.32) = 798 \quad T(3541.16) = 1496$   
 $\text{std error est} = 3 \quad \text{max error est} = 5$

CARBON (Atomic) C 300-1445K  
 $Cp(T) = 1750.3859 - 8.858597E-02T + 1.578577E-04T^2 - 1.2551E-07T^3$   
 $+ 3.676506E-11T^4$   
 $Cp(300) = 1734.93 \quad Cp(800) = 1731.34 \quad Cp(1445) = 1733.59$   
 $\text{std error est} = 0.52 \quad \text{max error est} = 1.0$   
 Note: For  $T(Cp)$  calculations, use the iterative procedures discussed  
 in Section 5 and the following eqn:  $300-1445K, Cp(T) = 1739.3435$   
 $- 0.018443T + 2.82288E-06T^2$

CARBON DIOXIDE  $CO_2$  200-1365K  
 Ideal gas  
 $Cp(T) = 453.86462 + 1.5334795T - 4.195556E-04T^2 - 1.871946E-06T^3$   
 $+ 2.862388E-09T^4 - 1.6962E-12T^5 + 3.717285E-16T^6$   
 $Cp(200) = 732.86 \quad Cp(800) = 1167.77 \quad Cp(1365) = 1308.13$   
 $\text{std error est} = 0.15 \quad \text{max error est} = 1.0$   
200-1365K  
 $T(Cp) = 10042.464 - 44.323467Cp + 7.31304E-02Cp^2 - 5.29105E-05Cp^3$   
 $+ 1.454422E-08Cp^4$   
 $T(732.86) = 206 \quad T(1167.77) = 798 \quad T(1308.13) = 1352$   
 $\text{std error est} = 4 \quad \text{max error est} = 14$

CARBON DIOXIDE - Real gas 200-1365K  
 $Cp(T) = 678.012 - 0.390396T + 6.23594E-03T^2 - 1.3596256E-05T^3$   
 $+ 1.3942973E-08T^4 - 7.036E-12T^5 + 1.40115E-15T^6$   
 $Cp(200) = 760.75 \quad Cp(800) = 1168.2 \quad Cp(1365) = 1310.6$   
 $\text{std error est} = 0.7 \quad \text{max error est} = 1.25$   
200-1365K  
 $T(Cp) = 7863.127 - 35.9779Cp + 6.10617E-02Cp^2 - 4.51148E-05Cp^3$   
 $+ 1.26481E-08Cp^4$



CARBON DIOXIDE - Real gas (continued)

T(760.75) = 205      T(1168.2) = 796      T(1310.6) = 1350  
 - std error est = 4.5 - - - - - max error est = 17 -  
 CARBON DISULFIDE CS<sub>2</sub>      100-1500K

Cp(T) = 234.3967 + 2.083974T - 4.080167E-03T<sup>2</sup> + 4.899365E-06T<sup>3</sup>  
          - 3.4779E-09T<sup>4</sup> + 1.329115E-12T<sup>5</sup> - 2.100283E-16T<sup>6</sup>  
 Cp(100) = 406.56      Cp(800) = 754.66      Cp(1500) = 809.08  
 - std error est = 0.9 - - - - - max error est = 2.0 -

CARBON MONOXIDE CO      255-1365K

Ideal gas

Cp(T) = 1020.802 + 0.382075T - 2.4945E-03T<sup>2</sup> + 6.81145E-06T<sup>3</sup>  
          - 7.93722E-09T<sup>4</sup> + 4.291972E-12T<sup>5</sup> - 8.903274E-16T<sup>6</sup>  
 Cp(255) = 1039.79      Cp(700) = 1113.16      Cp(1365) = 1242.76  
 std error est = 0.27      max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 255-1365K, Cp(T) = 1060.3 - 0.2338408T + 6.188684E-04T<sup>2</sup> - 2.584758E-07T<sup>3</sup>.

CARBON MONOXIDE - Real gas      275-1365K

Cp(T) = 1036.64564 + 0.2738793T - 2.16729E-03T<sup>2</sup> + 6.279075E-06T<sup>3</sup>  
          - 7.459832E-09T<sup>4</sup> + 4.072163E-12T<sup>5</sup> - 8.50011E-16T<sup>6</sup>  
 Cp(275) = 1042.02      Cp(700) = 1113.41      Cp(1365) = 1243.06  
 std error est = 0.26      max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the 3rd degree polynomial in the note above.

CARBON MONOSULFIDE CS      100-1500K

Cp(T) = 695.6713 - 0.590035T + 2.78573E-03T<sup>2</sup> - 4.25312E-06T<sup>3</sup>  
          + 3.1619707E-09T<sup>4</sup> - 1.16023E-12T<sup>5</sup> + 1.6791E-16T<sup>6</sup>  
 Cp(100) = 660.58      Cp(800) = 787.89      Cp(1500) = 833.81  
 - std error est = 1.1 - - - - - max error est = 2.0 -

CARBON SUBOXIDE C<sub>3</sub>O<sub>2</sub>      275-1500K

ln[Cp(T)] = 5.7661716 + 6.399978E-03T - 1.20235687E-05T<sup>2</sup>  
          + 1.16497649E-08T<sup>3</sup> - 5.5686458E-12T<sup>4</sup> + 1.03973134E-15T<sup>5</sup>  
 Cp(275) = 924.22      Cp(850) = 1377.47      Cp(1500) = 1533.42  
 - Note: Cp(T) = exp[fcn(T) above] - - - - - max error est = 36 -

CARBON TETRABROMIDE CBr<sub>4</sub>      300-1000K

Cp(T) = 195.977 + 0.3730265T - 3.99407E-04T<sup>2</sup> + 1.498015E-07T<sup>3</sup>  
 Cp(300) = 275.98      Cp(600) = 308.36      Cp(1000) = 319.4

## CARBON TETRABROMIDE (Continued)

std error est = 1.86

max error est = 3.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 300-1000K, Cp(T) =

$$228.26176 + 0.1975507T - 1.0812615E-04T^2$$

CARBON TETRACHLORIDE CCl<sub>4</sub> 100-700K

Ideal gas

$$Cp(T) = 104.89579 + 2.318459T - 2.59822E-03T^2 - 2.90876E-06T^3$$

$$+ 8.5781275E-09T^4 - 5.07917E-12T^5$$

$$Cp(100) = 308.66 \quad Cp(450) = 615.03 \quad Cp(700) = 662.94$$

std error est = 0.4

max error est = 1.0

$$Cp(T) = 458.4405 + 0.526876T - 4.11842E-04T^2 + 1.1014289E-07T^3$$

$$Cp(700) = 663.23 \quad Cp(1000) = 683.62 \quad Cp(1365) = 690.4$$

std error est = 0.2

max error est = 1.0

$$T(Cp) = 4845.83 - 45.40359Cp + 0.158658Cp^2 - 2.40639E-04Cp^3$$

$$+ 1.362815E-07Cp^4$$

$$T(308.66) = 108 \quad T(615.03) = 452 \quad T(662.94) = 686$$

std error est = 4.5

max error est = 14

Note: For T(Cp) calculations from 700-1365K, use the iterative procedures discussed in Section 5 and the following eqn: 700-

$$1365K, Cp(T) = 563.12016 + 0.198424T - 7.78963E-05T^2$$

CARBONYL CHLORIDE COCl<sub>2</sub> 100-1500K

FLUORIDE

$$Cp(T) = 309.8366 + 0.908395T + 2.14223E-03T^2 - 7.3825E-06T^3$$

$$+ 8.468816E-09T^4 - 4.393756E-12T^5 + 8.6745044E-16T^6$$

$$Cp(100) = 415.52 \quad Cp(800) = 884.22 \quad Cp(1500) = 965.61$$

std error est = 2.7 max error est = 4.5

CARBONYL FLUORIDE COF<sub>2</sub> 100-1500K

$$Cp(T) = 500.9343 - 0.685575T + 9.023284E-03T^2 - 1.958117E-05T^3$$

$$+ 1.949097E-08T^4 - 9.392863E-12T^5 + 1.769924E-15T^6$$

$$Cp(100) = 504.88 \quad Cp(800) = 1071.45 \quad Cp(1500) = 1195.03$$

std error est = 3.9 max error est = 7.5

CARBONYL SULFIDE COS 100-1500K

$$Cp(T) = 383.5831 + 1.008813T + 1.13734E-03T^2 - 5.397317E-06T^3$$

$$+ 6.74814E-09T^4 - 3.689623E-12T^5 + 7.566326E-16T^6$$

$$Cp(100) = 491.08 \quad Cp(800) = 908.47 \quad Cp(1500) = 1002.78$$

std error est = 3.2 max error est = 6.0

CHLORINE - Ideal gas  $\text{Cl}_2$  200-590K

$$\text{Cp}(T) = 333.73754 + 0.7763656T - 1.167902E-03T^2 + 6.302785E-07T^3$$

$\text{Cp}(200) = 447.34$        $\text{Cp}(400) = 497.76$        $\text{Cp}(590) = 514.69$   
 std error est = 0.15      max error est = 0.5

590-1365K

$$\text{Cp}(T) = 459.54857 + 0.1432384T - 9.84775E-05T^2 + 2.443506E-08T^3$$

$\text{Cp}(590) = 514.8$        $\text{Cp}(900) = 526.51$        $\text{Cp}(1365) = 533.73$   
 std error est = 0.14      max error est = 0.5

200-590K

$$T(\text{Cp}) = -164812.69 + 1056.14056\text{Cp} - 2.258534\text{Cp}^2 + 1.61435E-03\text{Cp}^3$$

$T(447.34) = 193$        $T(497.76) = 400$        $T(514.69) = 581$   
 std error est = 4.5      max error est = 12

Note: For  $T(\text{Cp})$  calculations from 590-1365K, use the iterative procedures discussed in Section 5 and the following eqn: 590-1365K,  $\text{Cp}(T) = 478.47124 + 7.90734E-02T - 2.858817E-05T^2$  . . . . .

CHLORINE (Atomic)  $\text{Cl}$  100-1500K

$$\text{Cp}(T) = 603.43652 - 0.43322T + 3.15819E-03T^2 - 7.17812E-06T^3$$

$$+ 7.4774E-09T^4 - 3.716555E-12T^5 + 7.151811E-16T^6$$

$\text{Cp}(100) = 585.23$        $\text{Cp}(800) = 635.29$        $\text{Cp}(1500) = 611.49$   
 std error est = 1.4      max error est = 2.5

Note: For  $T(\text{Cp})$  calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K,  $\text{Cp}(T) = 549.25664 + 0.326977T - 3.6189E-04T^2 + 1.145343E-07T^3$  . . . . .

CHLORINE DIOXIDE  $\text{ClO}_2$  100-1500K

$$\text{Cp}(T) = 474.2129 - 0.009513T + 3.445E-03T^2 - 7.92275E-06T^3$$

$$+ 7.90642E-09T^4 - 3.76735E-12T^5 + 6.99282E-16T^6$$

$\text{Cp}(100) = 500.54$        $\text{Cp}(800) = 802.25$        $\text{Cp}(1500) = 855.11$   
 std error est = 1.3      max error est = 2.5

CHLORINE FLUORIDE  $\text{ClF}$  250-1500K

$$\text{Cp}(T) = 415.24 + 0.88853T - 1.27775E-03T^2 + 9.74189E-07T^3$$

$$- 3.8041674E-10T^4 + 6.015904E-14T^5$$

$\text{Cp}(250) = 571.31$        $\text{Cp}(800) = 670.98$        $\text{Cp}(1500) = 691.96$   
 std error est = 0.4      max error est = 1.0

Note: For  $T(\text{Cp})$  calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K,  $\text{Cp}(T) = 464.27264 + 0.54434T - 4.614077E-04T^2 + 1.3377E-07T^3$  . . . . .

CHLORINE MONOXIDE  $\text{Cl}_2\text{O}$  100-1500K

$$\begin{aligned} \text{Cp}(T) &= 335.591265 + 0.654343T + 4.97567\text{E-}04T^2 - 2.93811\text{E-}06T^3 \\ &\quad + 3.65937\text{E-}09T^4 - 1.95317\text{E-}12T^5 + 3.902384\text{E-}16T^6 \\ \text{Cp}(100) &= 403.41 \quad \text{Cp}(900) = 640.62 \quad \text{Cp}(1500) = 659.25 \\ \text{std error est} &= 1.2 \quad \text{max error est} = 2.5 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K,  $\text{Cp}(T) = 329.537164 + 0.83896T - 7.41912\text{E-}04T^2 + 2.20666\text{E-}07T^3$ .

CHLORINE OXIDE  $\text{ClO}$  100-1500K

$$\begin{aligned} \text{Cp}(T) &= 591.2772 - 0.598616T + 4.16749\text{E-}03T^2 - 8.65076\text{E-}06T^3 \\ &\quad + 8.541837\text{E-}09T^4 - 4.10708\text{E-}12T^5 + 7.729816\text{E-}16T^6 \\ \text{Cp}(100) &= 565.25 \quad \text{Cp}(900) = 711.69 \quad \text{Cp}(1500) = 733.55 \\ \text{std error est} &= 1.5 \quad \text{max error est} = 3.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K,  $\text{Cp}(T) = 515.3754 + 0.426933T - 2.91036\text{E-}04T^2 + 6.836113\text{E-}08T^3$ .

CHLORINE TRIFLUORIDE  $\text{ClF}_3$  250-1500K

$$\begin{aligned} \text{Cp}(T) &= 80.2859 + 3.96595T - 9.1267\text{E-}03T^2 + 1.184492\text{E-}05T^3 \\ &\quad - 8.82973\text{E-}09T^4 + 3.5203\text{E-}12T^5 - 5.80698\text{E-}16T^6 \\ \text{Cp}(250) &= 655.24 \quad \text{Cp}(900) = 868.87 \quad \text{Cp}(1500) = 887.998 \\ \text{std error est} &= 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

CHLORODIFLUOROMETHANE  $\text{CHClF}_2$  90-645K

(FREON-22)- Ideal gas

$$\begin{aligned} \text{Cp}(T) &= 317.0722 + 0.514191T + 5.95107\text{E-}03T^2 - 2.58911\text{E-}05T^3 \\ &\quad + 6.22797\text{E-}08T^4 - 8.02754\text{E-}11T^5 + 4.084\text{E-}14T^6 \\ \text{Cp}(90) &= 396.31 \quad \text{Cp}(400) = 757.51 \quad \text{Cp}(645) = 935.32 \\ \text{std error est} &= 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

$$\begin{aligned} \text{Cp}(T) &= 276.0442 + 1.6021325T - 1.065933\text{E-}03T^2 + 2.585745\text{E-}07T^3 \\ \text{Cp}(645) &= 935.35 \quad \text{Cp}(900) = 1043.06 \quad \text{Cp}(1365) = 1134.52 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

$$\begin{aligned} \text{Cp}(T) &= 276.0442 + 1.6021325T - 1.065933\text{E-}03T^2 + 2.585745\text{E-}07T^3 \\ \text{Cp}(645) &= 935.35 \quad \text{Cp}(900) = 1043.06 \quad \text{Cp}(1365) = 1134.52 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

90-645K

$$\begin{aligned} T(\text{Cp}) &= 331.0157 - 3.35938\text{Cp} + 1.141036\text{E-}02\text{Cp}^2 - 1.36494\text{E-}05\text{Cp}^3 \\ &\quad + 6.06808\text{E-}09\text{Cp}^4 \\ T(396.31) &= 92 \quad T(757.51) = 399 \quad T(935.32) = 646 \\ \text{std error est} &= 1.3 \quad \text{max error est} = 3.5 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) &= 242225.509 - 986.8453\text{Cp} + 1.510484\text{Cp}^2 - 1.028665\text{E-}03\text{Cp}^3 \\ &\quad + 2.6358\text{E-}07\text{Cp}^4 \end{aligned}$$

CHLORODIFLUOROMETHANE (Continued)

T(935.35) = 644      T(1043.06) = 898      T(1134.52) = 1365  
 \_ std error est = 1 \_ \_ \_ \_ \_ max error est = 1 \_

CHLORODIFLUOROMETHANE,  $\text{CDClF}_2$       100-1000K  
 MONODEUTERATED

$\text{Cp}(T) = 355.67955 - 0.424395T + 1.121936E-02T^2 - 3.137704E-05T^3$   
 $+ 4.13097E-08T^4 - 2.71585E-11T^5 + 7.159286E-15T^6$   
 $\text{Cp}(100) = 397.92$        $\text{Cp}(600) = 938.49$        $\text{Cp}(1000) = 1084.09$   
 std error est = 0.6      max error est = 1.0

100-1000K  
 $T(\text{Cp}) = -2810.61 + 21.0917\text{Cp} - 6.179567E-02\text{Cp}^2 + 9.22238E-05\text{Cp}^3$   
 $- 6.82091E-08\text{Cp}^4 + 2.022326E-11\text{Cp}^5$   
 $T(397.92) = 100$        $T(938.49) = 598$        $T(1084.09) = 1000$   
 \_ std error est = 1.3 \_ \_ \_ \_ \_ max error est = 2.5

CHLOROFORM - Ideal gas       $\text{CHCl}_3$       100-755K

$\text{Cp}(T) = 189.1583 + 1.598713T - 1.340133E-03T^2 + 5.419056E-09T^3$   
 $+ 3.77955E-10T^4$   
 $\text{Cp}(100) = 335.67$        $\text{Cp}(500) = 677.78$        $\text{Cp}(755) = 757.42$   
 std error est = 0.2      max error est = 1.0

755-1365K  
 $\text{Cp}(T) = 402.7039 + 0.7755899T - 4.920244E-04T^2 + 1.152399E-07T^3$   
 $\text{Cp}(755) = 757.40$        $\text{Cp}(1000) = 801.51$        $\text{Cp}(1365) = 837.72$   
 std error est = 0.2      max error est = 1.0

100-755K  
 $T(\text{Cp}) = 1673.1583 - 14.61295\text{Cp} + 4.77988E-02\text{Cp}^2 - 6.568945E-05\text{Cp}^3$   
 $+ 3.424226E-08\text{Cp}^4$   
 $T(335.67) = 104$        $T(677.78) = 500$        $T(757.42) = 753$   
 std error est = 1.8      max error est = 3.5

755-1365K  
 $T(\text{Cp}) = -179838.72 + 710.17532\text{Cp} - 0.936808\text{Cp}^2 + 4.14539E-04\text{Cp}^3$   
 $T(757.40) = 755$        $T(801.51) = 1000$        $T(837.72) = 1365$   
 \_ std error est = 0.8 \_ \_ \_ \_ \_ max error est = 2.5

CHLOROFLUOROMETHANE       $\text{CH}_2\text{ClF}$       200-1000K

$\text{Cp}(T) = 638.4166 - 2.34596T + 1.549633E-02T^2 - 3.2233E-05T^3$   
 $+ 3.40267E-08T^4 - 1.8304265E-11T^5 + 3.978875E-15T^6$   
 $\text{Cp}(200) = 580.05$        $\text{Cp}(600) = 1019.35$        $\text{Cp}(1000) = 1257.1$   
 std error est = 0.4      max error est = 1.0

200-1000K  
 $T(\text{Cp}) = -1079.2262 + 4.074\text{Cp} - 4.3312E-03\text{Cp}^2 + 1.912603E-06\text{Cp}^3$   
 $T(580.05) = 200$        $T(1019.35) = 599$        $T(1257.1) = 997$   
 \_ std error est = 1.4 \_ \_ \_ \_ \_ max error est = 3 \_

CHLOROMETHYLIDYNE CC1 300-1500K

$$Cp(T) = 543.19413 + 0.651587T - 7.2857E-04T^2 + 3.84102E-07T^3 - 7.77988E-11T^4$$

Cp(300) = 682.84      Cp(800) = 762.97      Cp(1500) = 783.78  
std error est = 0.4      max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 300-1500K, Cp(T) = 570.92334 + 0.48166T - 3.8583E-04T<sup>2</sup> + 1.066284E-07T<sup>3</sup> - - - - -

CHLOROSILANE SiH<sub>3</sub>Cl 100-1000K

$$Cp(T) = 632.108 - 3.352308T + 2.6872E-02T^2 - 7.054946E-05T^3 + 9.37112E-08T^4 - 6.27597E-11T^5 + 1.67893E-14T^6$$

Cp(100) = 503.81      Cp(500) = 1013.31      Cp(1000) = 1343.14  
std error est = 1.6      max error est = 3.0

CHLOROTRIFLUOROMETHANE CC1F<sub>3</sub> 200-1090K

(FREON-13) - Ideal gas

$$Cp(T) = 77.23115 + 2.79399T - 3.680032E-03T^2 + 2.4349E-06T^3 - 6.56569E-10T^4$$

Cp(200) = 507.26      Cp(600) = 869.66      Cp(1090) = 976.9  
std error est = 0.3      max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 200-1090, Cp(T) = 137.21148 + 2.290486T - 2.25364E-03T<sup>2</sup> + 7.92858E-07T<sup>3</sup> - - - - -

CUMENE C<sub>6</sub>H<sub>5</sub>CH(CH<sub>3</sub>)<sub>2</sub> 275-1500K

$$Cp(T) = 80.85313 + 2.55483T + 1.017634E-02T^2 - 2.428585E-05T^3 + 2.32E-08T^4 - 1.05785E-11T^5 + 1.8904E-15T^6$$

Cp(275) = 1164.81      Cp(800) = 2735.13      Cp(1500) = 3497.47  
std error est = 1.7      max error est = 5

275-1500K

$$T(Cp) = 622.8356 - 1.098344Cp + 1.04225E-03Cp^2 - 3.612275E-07Cp^3 + 4.95368E-11Cp^4$$

T(1164.81) = 278      T(2735.13) = 797      T(3497.47) = 1489  
std error est = 4.0      max error est = 14

CYANOGEN (CN)<sub>2</sub> 100-1500K

$$Cp(T) = 311.4587 + 4.93727T - 1.16917E-02T^2 + 1.6521E-05T^3 - 1.31327E-08T^4 + 5.4334E-12T^5 - 9.1145E-16T^6$$

Cp(100) = 703.53      Cp(800) = 1399.67      Cp(1500) = 1563.02  
std error est = 1.2      max error est = 2.5

CYANOGEN CHLORIDE      CNC1      100-1500K

$$Cp(T) = 287.6997 + 2.740703T - 6.197496E-03T^2 + 8.19973E-06T^3 - 6.1265E-09T^4 + 2.39758E-12T^5 - 3.82468E-16T^6$$

$$Cp(100) = 507.41 \quad Cp(800) = 888.09 \quad Cp(1500) = 963.14$$

$$\text{std error est} = 1.1 \quad \text{max error est} = 2.5$$

CYCLOHEXANE - See HEXANE

CYCLOPROPANE - See PROPANE

n-DECANE - Ideal gas      C<sub>10</sub>H<sub>22</sub>      300-700K

$$Cp(T) = 240.7178 + 5.09965T - 6.29026E-04T^2 - 1.07155E-06T^3$$

$$Cp(300) = 1685.07 \quad Cp(500) = 2499.34 \quad Cp(700) = 3134.71$$

$$\text{std error est} = 0.1 \quad \text{max error est} = 1.0$$

700-1365K

$$Cp(T) = -13534.589 + 91.4879T - 0.2207T^2 + 2.91406E-04T^3$$

$$- 2.153074E-07T^4 + 8.386E-11T^5 - 1.34404E-14T^6$$

$$Cp(700) = 3134.09 \quad Cp(1000) = 3771.91 \quad Cp(1365) = 4258.15$$

$$\text{std error est} = 1.2 \quad \text{max error est} = 2.0$$

300-700K

$$T(Cp) = -201.2556 + 0.4224556Cp - 1.10665E-04Cp^2 + 2.15458E-08Cp^3$$

$$T(1685.07) = 299 \quad T(2499.34) = 500 \quad T(3134.71) = 699$$

$$\text{std error est} = 0.3 \quad \text{max error est} = 1$$

700-1365K

$$T(Cp) = 11052.013 - 13.05146Cp + 5.9256E-03Cp^2 - 1.1798E-06Cp^3 + 8.983E-11Cp^4$$

$$T(3134.09) = 699 \quad T(3771.91) = 998 \quad T(4258.15) = 1362$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 3$$

n-DEUTERIUM      D<sub>2</sub>      200-645K

Ideal gas

$$Cp(T) = 7264.2197 + 0.037477T - 7.05335E-04T^2 + 1.51166E-06T^3$$

$$Cp(200) = 7255.6 \quad Cp(400) = 7264.28 \quad Cp(645) = 7400.59$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.0$$

645-1365K

$$Cp(T) = 7583.3708 - 2.017012T + 3.3723E-03T^2 - 1.080913E-06T^3$$

$$Cp(645) = 7395.31 \quad Cp(1000) = 7857.75 \quad Cp(1365) = 6364.41$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.0$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqns: 200-645K, Cp(T) = 7353.022 - 0.72328T + 1.2086E-03T<sup>2</sup>; 645-1365K, Cp(T) = 6629.115 + 1.06105T + 1.642087E-04T<sup>2</sup>.

DEUTERIUM ( Monatomic) D 55-1500K

- Cp(T) = 10.32 = constant - - - - -

DIBROMOMETHANE CH<sub>2</sub>Br<sub>2</sub> 300-1000K

$$\begin{aligned} \text{Cp}(T) &= 104.624 + 0.911614T - 7.67807E-04T^2 + 2.58695E-07T^3 \\ \text{Cp}(300) &= 315.99 \quad \text{Cp}(600) = 431.06 \quad \text{Cp}(1000) = 507.13 \\ \text{std error est} &= 0.3 \quad \text{max error est} = 1.0 \end{aligned}$$

300-1000K

$$\begin{aligned} T(\text{Cp}) &= -2029.747 + 17.57971\text{Cp} - 4.78704E-02\text{Cp}^2 + 4.927377E-05\text{Cp}^3 \\ T(315.99) &= 300 \quad T(431.06) = 600 \quad T(507.13) = 1001 \\ \text{std error est} &= 0.7 \quad \text{max error est} = 1.5 \end{aligned}$$

DICHLORODIFLUOROMETHANE 100-1365K CCl<sub>2</sub>F<sub>2</sub>

(FREON-12) - Ideal gas

$$\begin{aligned} \text{Cp}(T) &= 115.7338 + 2.37887T - 2.812186E-03T^2 + 5.571888E-07T^3 \\ &\quad + 1.82207E-09T^4 - 1.6317E-12T^5 + 4.2395E-16T^6 \\ \text{Cp}(100) &= 326.22 \quad \text{Cp}(800) = 827.04 \quad \text{Cp}(1365) = 875.74 \\ \text{std error est} &= 0.3 \quad \text{max error est} = 1.0 \end{aligned}$$

1,1-DICHLORO-1-FLUORO-ETHANE 300-600K CH<sub>3</sub>CFC1<sub>2</sub>

$$\text{Cp}(T) = 474 + 1.0T \quad T(\text{Cp}) = \text{Cp} - 474$$

Note: There are only three (3) data points available from the reference source. The accuracy cannot be adequately established.

DICHLOROFLUOROMETHANE 100-755K CHCl<sub>2</sub>F

(FREON-21) - Ideal gas

$$\begin{aligned} \text{Cp}(T) &= 209.72 + 1.79069T - 3.45786E-03T^2 + 1.0810155E-05T^3 \\ &\quad - 2.22979E-08T^4 + 2.16214E-11T^5 - 7.79904E-15T^6 \\ \text{Cp}(100) &= 362.999 \quad \text{Cp}(450) = 720.25 \quad \text{Cp}(755) = 857.42 \\ \text{std error est} &= 0.3 \quad \text{max error est} = 1.0 \end{aligned}$$

755-1365K

$$\begin{aligned} \text{Cp}(T) &= 388.2867 + 1.023759T - 6.4682E-04T^2 + 1.50429E-07T^3 \\ \text{Cp}(755) &= 857.26 \quad \text{Cp}(1000) = 915.65 \quad \text{Cp}(1365) = 963.13 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

100-755K

$$\begin{aligned} T(\text{Cp}) &= 921.3768 - 7.7154\text{Cp} + 2.414285E-02\text{Cp}^2 - 3.033265E-05\text{Cp}^3 \\ &\quad + 1.446893E-08\text{Cp}^4 \\ T(362.99) &= 102 \quad T(720.25) = 449 \quad T(857.42) = 755 \\ \text{std error est} &= 1.1 \quad \text{max error est} = 2.0 \end{aligned}$$

755-1365K

$$\begin{aligned} T(\text{Cp}) &= -122177 + 424.7354\text{Cp} - 0.493077\text{Cp}^2 + 1.923554E-04\text{Cp}^3 \\ T(857.26) &= 755 \quad T(915.65) = 999 \quad T(963.13) = 1364 \\ \text{std error est} &= 1.1 \quad \text{max error est} = 2.0 \end{aligned}$$



DICHLOROFLUOROMETHANE, 100-1000K  $\text{CDCl}_2\text{F}$   
MONODEUTERATED

$$\text{Cp}(T) = 255.720254 + 0.689369T + 4.583258E-03T^2 - 1.3455115E-05T^3 \\ + 1.377348E-08T^4 - 4.9189282E-12T^5$$

$$\text{Cp}(100) = 358.36 \quad \text{Cp}(500) = 771.46 \quad \text{Cp}(1000) = 927.78$$

$$\text{std error est} = 5.8 \quad \text{max error est} = 10$$

DICHLOROMETHANE  $\text{CH}_2\text{Cl}_2$  275-1500K

$$\text{Cp}(T) = 132.0712 + 2.141377T - 2.08642E-03T^2 + 1.059563E-06T^3 \\ - 2.15869E-10T^4$$

$$\text{Cp}(275) = 583.97 \quad \text{Cp}(800) = 963.94 \quad \text{Cp}(1500) = 1132.88 \\ \text{std error est} = 0.9 \quad \text{max error est} = 2.0$$

275-1500K

$$T(\text{Cp}) = 5523.4 - 29.33479\text{Cp} + 5.93745E-02\text{Cp}^2 - 5.22736E-05\text{Cp}^3 \\ + 1.760695E-08\text{Cp}^4$$

$$T(583.97) = 278 \quad T(963.94) = 797 \quad T(1132.88) = 1491$$

$$\text{std error est} = 5.0 \quad \text{max error est} = 9$$

1,1-DICHLOROTETRAFLUORO- 275-600K  $\text{CCl}_2\text{FCF}_3$   
ETHANE

$$\text{Cp}(T) = -104.2484 + 4.520335T - 8.19256E-03T^2 + 5.7332E-06T^3$$

$$\text{Cp}(275) = 638.51 \quad \text{Cp}(450) = 793.35 \quad \text{Cp}(600) = 897.00$$

$$\text{std error est} = 0.01 \quad \text{max error est} = 0.5$$

275-600K

$$T(\text{Cp}) = 421.358 - 1.292708\text{Cp} + 1.66326E-03\text{Cp}^2$$

$$T(638.51) = 274 \quad T(793.35) = 443 \quad T(897.00) = 600$$

$$\text{std error est} = 1.4 \quad \text{max error est} = 2.5$$

DICHLOROTETRAFLUORO- 220-510K  $\text{C}_2\text{Cl}_2\text{F}_4$   
ETHANE (FREON-114)

$$\text{Cp}(T) = -94.71864 + 4.57011T - 7.699598E-03T^2 + 4.89705E-06T^3$$

$$\text{Cp}(220) = 590.19 \quad \text{Cp}(400) = 814.8 \quad \text{Cp}(510) = 882.97$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.0$$

220-510K

$$T(\text{Cp}) = -1652.37 + 7.94254\text{Cp} - 1.184297E-02\text{Cp}^2 + 6.36623E-06\text{Cp}^3$$

$$T(590.19) = 219 \quad T(814.8) = 400 \quad T(882.97) = 510$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

2,2-DICHLORO-1,1,1-TRI- 200-800K  $\text{F}_3\text{CCHCl}_2$   
FLUOROETHANE

$$\text{Cp}(T) = 1319.2995 - 14.01811T + 8.407976E-02T^2 - 2.15252E-04T^3 \\ + 2.57008E-07T^4 - 1.15831E-10T^5$$

$$\text{Cp}(200) = 530.999 \quad \text{Cp}(500) = 866.97 \quad \text{Cp}(800) = 1021.81$$

$$\text{std error} = 0.5 \quad \text{max error est} = 2.5^*$$

\*Note:  $\text{Cp}(700) = 1114.17$  but table value is 984.

1,1-DIFLUOROETHYLENE  $\text{CH}_2\text{CF}_2$  175-1175K

$$\text{Cp}(T) = 472.82 - 1.09967T + 1.798667E-02T^2 - 4.64504E-05T^3 \\ + 5.802696E-08T^4 - 3.622937E-11T^5 + 8.981685E-15T^6$$

$$\text{Cp}(175) = 631.01 \quad \text{Cp}(600) = 1377.09 \quad \text{Cp}(1175) = 1760.59$$

$$\text{std error est} = 4.4 \quad \text{max error est} = 8$$

DIFLUOROMETHANE  $\text{CH}_2\text{F}_2$  200-1000K

$$\text{Cp}(T) = 926.6998 - 4.228109T + 2.28603E-02T^2 - 4.39433E-05T^3 \\ + 4.39172E-08T^4 - 2.27523E-11T^5 + 4.84046E-15T^6$$

$$\text{Cp}(200) = 707.24 \quad \text{Cp}(500) = 1144.26 \quad \text{Cp}(1000) = 1620.95$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1.0$$

200-1000K

$$T(\text{Cp}) = -1024.354 + 3.046388\text{Cp} - 2.430315E-03\text{Cp}^2 + 8.15023E-07\text{Cp}^3$$

$$T(707.24) = 203 \quad T(1144.26) = 500 \quad T(1620.95) = 999$$

$$\text{std error est} = 1.5 \quad \text{max error est} = 3.5$$

DIMETHYLAMINE  $(\text{CH}_3)_2\text{NH}$  275-1475K

$$\text{Cp}(T) = 843.8386 - 1.4191273T + 2.18139E-02T^2 - 4.059054E-05T^3 \\ + 3.603484E-08T^4 - 1.5961557E-11T^5 + 2.82084E-15T^6$$

$$\text{Cp}(275) = 1441.30 \quad \text{Cp}(800) = 3156.13 \quad \text{Cp}(1475) = 4128.28$$

$$\text{std error est} = 2.4 \quad \text{max error est} = 4.5$$

275-1475K

$$T(\text{Cp}) = 389.02765 - 0.587004715\text{Cp} + 5.4705492E-04\text{Cp}^2 - 1.6211353E-07\text{Cp}^3 \\ + 1.92366E-11\text{Cp}^4$$

$$T(1441.30) = 277 \quad T(3156.13) = 798 \quad T(4128.28) = 1471$$

$$\text{std error est} = 3.5 \quad \text{max error est} = 6$$

2,2-DIMETHYLBUTANE  $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2$  300-1000K

$$\text{Cp}(T) = 2581.4188 - 21.863667T + 0.11908912T^2 - 2.667096E-04T^3 \\ + 3.179459E-07T^4 - 1.9721679E-10T^5 + 5.005353E-14T^6$$

$$\text{Cp}(300) = 1671.79 \quad \text{Cp}(600) = 2931.54 \quad \text{Cp}(1000) = 3879.91$$

$$\text{std error est} = 1.8 \quad \text{max error est} = 2.5$$

300-1000K

$$T(\text{Cp}) = -245.69753 + 0.521407\text{Cp} - 1.6592016E-04\text{Cp}^2 + 2.9471092E-08\text{Cp}^3$$

$$T(1671.79) = 300 \quad T(2931.54) = 599 \quad T(3879.91) = 1001$$

$$\text{std error est} = 1.6 \quad \text{max error est} = 2.5$$

2,3-DIMETHYLBUTANE  $[(\text{CH}_3)_2\text{CH}]_2$  300-1000K

$$\text{Cp}(T) = 734.10753 - 0.560625T + 2.23453E-02T^2 - 4.17216E-05T^3 \\ + 3.25804E-08T^4 - 9.52277E-12T^5$$

$$\text{Cp}(300) = 1691.27 \quad \text{Cp}(600) = 2912.1 \quad \text{Cp}(1000) = 3854.81$$

$$\text{std error est} = 2.2 \quad \text{max error est} = 4.5$$

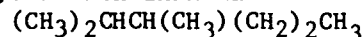
2,3-DIMETHYLBUTANE (Continued) 300-1000K

$$T(Cp) = -218.0723 + 0.473152Cp - 1.438724E-04Cp^2 + 2.6738645E-08Cp^3$$

$$T(1691.27) = 300 \quad T(2912.1) = 600 \quad T(3854.81) = 1000$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 1.5$$

2,3-DIMETHYLHEXANE 395-520K

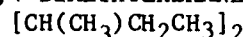


$$Cp(T) = 605.9 + 3.8822T \quad T(Cp) = [Cp - 605.9]/3.8822$$

Note: There are only three data points in the reference source.

The accuracy of the fits cannot be adequately estimated.

3,4-DIMETHYLHEXANE 405-520K



$$Cp(T) = 594.01 + 3.881T \quad T(Cp) = [Cp - 594.01]/3.881$$

Note: There are only three data points in the reference source.

The accuracy of the fits cannot be adequately estimated.

DIMETHYLPROPANE  $C(CH_3)_4$  300-1500K

$$\ln[Cp(T)] = 6.1724277 + 5.9032424E-03T - 6.648126E-06T^2 \\ + 3.6018484E-09T^3 - 7.508868E-13T^4$$

$$**Cp(T) = \exp[fctn(T)]$$

$$Cp(300) = 1696.35 \quad Cp(800) = 3557.47 \quad Cp(1500) = 4554.55$$

$$\text{std error est} = 8.00674E-03 \text{ for } \ln[Cp(T)]$$

DIPROPYLENE GLYCOL  $(CH_3CHOHCH_2)_2O$  275-775K

$$Cp(T) = -1826.75484 + 36.04835T - 0.1900801T^2 + 5.610031E-04T^3$$

$$-9.03165E-07T^4 + 7.46426E-10T^5 - 2.482783E-13T^6$$

$$Cp(275) = 1280.09 \quad Cp(500) = 1801.43 \quad Cp(775) = 2155.97$$

$$\text{std error est} = 2.8 \quad \text{max error est} = 3.5$$

275-775K

$$T(Cp) = -395.8809 + 0.389689Cp + 5.172082E-04Cp^2 - 4.901004E-07Cp^3 \\ + 1.31177E-10Cp^4$$

$$T(1280.09) = 275 \quad T(1801.43) = 501 \quad T(2155.97) = 771$$

$$\text{std error est} = 2.4 \quad \text{max error est} = 5$$

DODECANE  $CH_3(CH_2)_{10}CH_3$  300-1500K

$$Cp(T) = 827.74543 - 0.177414T + 1.89547E-02T^2 - 3.681404E-05T^3$$

$$+ 3.299875E-08T^4 - 1.45863E-11T^5 + 2.55543E-15T^6$$

$$Cp(300) = 1720.17 \quad Cp(800) = 3374.57 \quad Cp(1500) = 4361.72$$

$$\text{std error est} = 5.0 \quad \text{max error est} = 7.5$$

300-1500K

$$T(Cp) = 867.5699 - 1.28664Cp + 8.801372E-04Cp^2 - 2.28373E-07Cp^3 \\ + 2.333242E-11Cp^4$$

$$T(1720.17) = 301 \quad T(3374.57) = 798 \quad T(4361.72) = 1496$$

$$\text{std error est} = 4.5 \quad \text{max error est} = 7.5$$

ETHANE - Ideal gas  $C_2H_6$  275-755K

$$Cp(T) = 531.9795 + 3.755877T + 1.789289E-03T^2 - 2.13225E-06T^3$$

$Cp(275) = 1655.82$        $Cp(500) = 2590.71$        $Cp(755) = 3469.95$   
 std error est = 0.1      max error est = 1.0

755-1365K

$$Cp(T) = 3718.3729 - 10.891558T + 2.95115E-02T^2 - 2.95597E-05T^3$$

$$+ 1.382794E-08T^4 - 2.52553E-12T^5$$

$Cp(755) = 3469.49$        $Cp(1000) = 4081.02$        $Cp(1365) = 4696.05$   
 std error est = 0.4      max error est = 1.0

275-755K

$$T(Cp) = 26.69485 - 0.0209973Cp + 1.77038E-04Cp^2 - 5.60605E-08Cp^3$$

$$+ 6.976759E-12Cp^4$$

$T(1655.82) = 275$        $T(2590.71) = 500$        $T(3469.95) = 755$   
 std error est = 0.2      max error est = 1

755-1365K

$$T(Cp) = -3405.9176 + 2.9438457Cp - 7.63789E-04Cp^2 + 7.521499E-08Cp^3$$

$T(3469.49) = 755$        $T(4081.02) = 1000$        $T(4696.05) = 1364$   
 std error est = 0.5      max error est = 1.5

ETHANE , HEXADEUTERATED  $C_2D_6$  275-365K

$$Cp(T) = 1100.6747 - 3.438783T + 2.9385375E-02T^2 - 3.3966273E-05T^3$$

$Cp(275) = 1670.89$        $Cp(315) = 1871.58$        $Cp(365) = 2108.7$   
 std error est = 0.1      max error est = 1.0

Note: For  $T(Cp)$  calculations, use the iterative procedures discussed in Section 5 and the polynomial above.

ETHANETHIOL  $C_2H_5SH$  300-1000K

$$Cp(T) = 357.285 + 2.59852T + 1.61883E-03T^2 - 4.13005E-06T^3$$

$$+ 1.930025E-09T^4$$

$Cp(300) = 1186.66$        $Cp(700) = 2016.27$        $Cp(1000) = 2374.61$   
 std error est = 5.5      max error est = 9.5

300-1000K

$$T(Cp) = -340.822 + 0.8964337Cp - 4.606323E-04Cp^2 + 1.352216E-07Cp^3$$

$T(1186.66) = 300$        $T(2016.27) = 702$        $T(2374.61) = 1001$   
 std error est = 4.8      max error est = 6.5

ETHYL ACETATE  $CH_3COOCH_2CH_3$  370-440K

$$Cp(T) = -1312.0132 + 11.8064T - 1.1402197E-02T^2$$

$Cp(370) = 1495.39$        $Cp(400) = 1586.2$        $Cp(440) = 1675.34$   
 std error est = 8.3      max error est = 15

Note: For  $T(Cp)$  calculations, use the iterative procedures discussed in Section 5 and the equation above. The  $T(Cp)$  calculations may not agree well due to the std error ests above.

ETHYL ALCOHOL  $C_2H_5OH$  255-810K

Ideal gas

$$Cp(T) = 546.2212 + 3.8600396T - 1.023837E-03T^2 - 2.75659E-07T^3$$

$$Cp(255) = 1459.39 \quad Cp(500) = 2185.82 \quad Cp(810) = 2854.62$$

$$std \ error \ est = 0.3 \quad \quad \quad max \ error \ est = 1.5$$

810-1365K

$$Cp(T) = 835.49557 + 3.1089285T - 4.372953E-04T^2 - 5.607147E-07T^3 + 2.0162334E-10T^4$$

$$Cp(810) = 2855.62 \quad Cp(1100) = 3275.08 \quad Cp(1365) = 3538.29$$

$$std \ error \ est = 0.2 \quad \quad \quad max \ error \ est = 1.0$$

255-810K

$$T(Cp) = -394.5867 + 0.668288Cp - 2.236847E-04Cp^2 + 4.805682E-08Cp^3$$

$$T(1459.39) = 254 \quad T(2185.82) = 499 \quad T(2854.62) = 808$$

$$std \ error \ est = 0.7 \quad \quad \quad max \ error \ est = 2$$

810-1365K

$$T(Cp) = -7130.17 + 7.512807Cp - 2.545385E-03Cp^2 + 3.11057E-07Cp^3$$

$$T(2855.62) = 810 \quad T(3275.08) = 1100 \quad T(3538.29) = 1364$$

$$- \quad std \ error \ est = 0.2 \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad max \ error \ est = 2 \quad - \quad - \quad - \quad - \quad - \quad - \quad -$$

ETHYLBENZENE  $C_6H_5C_2H_5$  275-1500K

$$Cp(T) = 88.81893 + 2.2813924T + 1.0434866E-02T^2 - 2.431028E-05T^3 + 2.3069044E-08T^4 - 1.0491076E-11T^5 + 1.87293E-15T^6$$

$$Cp(275) = 1116.01 \quad Cp(800) = 2647.73 \quad Cp(1500) = 3396.43$$

$$std \ error \ est = 1.9 \quad \quad \quad max \ error \ est = 6$$

275-1500K

$$T(Cp) = 642.15192 - 1.1750234Cp + 1.1452373E-03Cp^2 - 4.0876E-07Cp^3 + 5.746896E-11Cp^4$$

$$T(1116.01) = 278 \quad T(2647.73) = 797 \quad T(3396.43) = 1495$$

$$- \quad std \ error \ est = 3.9 \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad max \ error \ est = 8 \quad - \quad - \quad - \quad - \quad - \quad - \quad -$$

ETHYL ETHER  $C_4H_{10}O$  310-600K

$$Cp(T) = -4053.47326 + 33.471276T - 6.7641844E-02T^2 + 5.094208E-05T^3$$

$$Cp(310) = 1339.87 \quad Cp(450) = 1953.22 \quad Cp(600) = 2681.72$$

$$std \ error \ est = 0.2 \quad \quad \quad max \ error \ est = 1.0$$

310-600K

$$T(Cp) = 779.23434 - 1.052998Cp + 6.81429E-04Cp^2 - 1.17146E-07Cp^3$$

$$T(1339.87) = 310 \quad T(1953.22) = 449 \quad T(2681.72) = 597$$

$$- \quad std \ error \ est = 1.5 \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad max \ error \ est = 3 \quad - \quad - \quad - \quad - \quad - \quad - \quad -$$

ETHYLENE - Ideal gas  $C_2H_4$  275-755K

$$Cp(T) = 248.817245 + 4.864076T - 1.570483E-03T^2 - 2.3772E-07T^3$$

$$Cp(275) = 1462.73 \quad Cp(500) = 2258.52 \quad Cp(755) = 2923.67$$

$$std \ error \ est = 0.2 \quad \quad \quad max \ error \ est = 1.0$$

ETHYLENE - Ideal gas (continued) 755-1365K

$$C_p(T) = 883.873 + 2.982773T + 2.684874E-04T^2 - 1.103103E-06T^3 + 3.3579064E-10T^4$$

$$C_p(755) = 2923.28 \quad C_p(1000) = 3367.82 \quad C_p(1365) = 3815.82$$

$$\text{std error est} = 0.3 \quad \text{max error est} = 1.0$$

275-755K

$$T(C_p) = -215.2115 + 0.46972C_p - 1.376816E-04C_p^2 + 3.0917277E-08C_p^3$$

$$T(1462.73) = 274 \quad T(2258.52) = 500 \quad T(2923.67) = 754$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 2$$

755-1365K

$$T(C_p) = -4851.525 + 4.91917C_p - 1.56526E-03C_p^2 + 1.842345E-07C_p^3$$

$$T(2923.28) = 755 \quad T(3367.82) = 999 \quad T(3815.82) = 1364$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1$$

ETHYLENE - Real gas 275-610K

$$C_p(T) = 452.40453 + 3.594527T + 1.099394E-03T^2 - 2.103391E-06T^3$$

$$C_p(275) = 1480.3 \quad C_p(450) = 2100.9 \quad C_p(610) = 2576.72$$

$$\text{std error est} = 1.5 \quad \text{max error est} = 2.5$$

Note: For  $T(C_p)$  calculations, use the iterative procedures discussed in Section 5 and the polynomial immediately above.

ETHYLENE OXIDE  $(CH_2)_2O$  275-1000K

$$C_p(T) = 1405.23696 - 8.747353T + 4.235163E-02T^2 - 6.972269E-05T^3 + 5.2382475E-08T^4 - 1.5060405E-11T^5$$

$$C_p(275) = 1028.44 \quad C_p(600) = 1960.98 \quad C_p(1000) = 2608.89$$

$$\text{std error est} = 5.0 \quad \text{max error est} = 7.5$$

275-1365K

$$T(C_p) = -324.12166 + 0.929479C_p - 4.506574E-04C_p^2 + 1.107183E-07C_p^3$$

$$T(1028.44) = 276 \quad T(1960.98) = 600 \quad T(2608.89) = 999$$

$$\text{std error est} = 1.5 \quad \text{max error est} = 3$$

3-ETHYLHEXANE  $(CH_3CH_2)_2CH(CH_2)_2CH_3$  295-520K

$$C_p(T) = 1559.9 + 1.928T \quad T(C_p) = [C_p - 1559.9]/1.928$$

Note: There are only three data points in the reference source.  
The accuracy of the fit cannot be adequately established.

3-ETHYL-2-METHYL- PENTANE  $(CH_3)_2CHCH(C_2H_5)_2$  400-520K

$$C_p(T) = 658.8 + 3.7806T \quad T(C_p) = [C_p - 658.8]/3.7806$$

Note: There are only three data points in the reference source.  
The accuracy of the fit cannot be adequately established.

3-ETHYL-3-METHYL- PENTANE  $(CH_3CH_2)_3CCH_3$  400-520K

$$C_p(T) = 641.9 + 3.8767T \quad T(C_p) = [C_p - 641.9]/3.8767$$

Note: There are only three data points in the reference source.  
The accuracy of the fit cannot be adequately established.

FLUORINE  $F_2$  200-645K  
 Ideal gas  
 $C_p(T) = 658.25722 + 0.6751476T - 3.79745E-04T^2 + 2.235484E-09T^3$   
 $C_p(200) = 778.11$   $C_p(450) = 885.38$   $C_p(645) = 936.34$   
 std error est = 0.01 max error est = 1.0  
645-1365K  
 $C_p(T) = 127.23948 + 3.72368T - 7.033226E-03T^2 + 6.867834E-06T^3$   
 $- 3.366543E-09T^4 + 6.5637923E-13T^5$   
 $C_p(645) = 936.51$   $C_p(1000) = 975.36$   $C_p(1365) = 995.65$   
 std error est = 0.3 max error est = 1.0  
200-645K  
 $T(C_p) = 3954.34 - 11.05956C_p + 8.024798E-03C_p^2$   
 $T(778.11) = 207$   $T(885.38) = 453$   $T(936.34) = 634$   
 std error est = 5.0 max error est = 11  
645-1365K  
 $T(C_p) = 112357.756 - 242.565496C_p + 0.131647C_p^2$   
 $T(936.51) = 654$   $T(975.36) = 1008$   $T(995.65) = 1351$   
 std error est = 7.5 max error est = 15.5  
 - - - - -  
 FLUORINE (Monatomic)  $F$  100-1500K  
 $C_p(T) = 925.04634 + 2.7925687T - 1.038958E-02T^2 + 1.78943E-05T^3$   
 $- 1.6070342E-08T^4 + 7.28505E-12T^5 - 1.315903E-15T^6$   
 $C_p(100) = 1116.77$   $C_p(800) = 1131.45$   $C_p(1500) = 1106.39$   
 std error est = 1.7 max error est = 3.5  
 - - - - -  
 FLUOROETHANE  $CH_3CH_2F$  100-1500K  
 $\ln[C_p(T)] = 6.471145519 + 2.09924177E-03T + 1.99348096E-06T^2$   
 $- 5.55076164E-09T^3 + 3.8054008E-12T^4 - 8.6180454E-16T^5$   
 $C_p(100) = 809.02$   $C_p(800) = 2593.26$   $C_p(1500) = 3268.33$   
 std error est = 10.0 max error est = 85  
 \*\*Note:  $C_p(T) = \exp[fcfn(T)]$   
 - - - - -  
 FLUOROETHYLENE  $CH_2CHF$  175-975K  
 $C_p(T) = 580.68945 - 1.7973376T + 2.027156E-02T^2 - 4.167712E-05T^3$   
 $+ 3.705407E-08T^4 - 1.2304487E-11T^5$   
 $C_p(175) = 696.34$   $C_p(600) = 1643.20$   $C_p(975) = 2113.99$   
 std error est = 7.1 max error est = 13.5  
175-975K  
 $T(C_p) = -171.8982 + 0.671097C_p - 3.337414E-04C_p^2 + 1.285454E-07C_p^3$   
 $T(696.34) = 177$   $T(1643.20) = 600$   $T(2113.99) = 970$   
 std error est = 5.5 max error est = 10  
 - - - - -

FLUOROFORM, MONODEUTERATED  $\text{CF}_3\text{D}$  100-1000K

$$\begin{aligned} \text{Cp}(T) = & 529.7845 - 1.9731807T + 1.8510456E-02T^2 - 4.45372E-05T^3 \\ & + 5.268778E-08T^4 - 3.146596E-11T^5 + 7.57734E-15T^6 \\ \text{Cp}(100) = & 477.99 \quad \text{Cp}(600) = 1124.68 \quad \text{Cp}(1000) = 1329.02 \\ \text{std error est} = & 0.6 \quad \text{max error est} = 1.0 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) = & -134.042 - 0.440011\text{Cp} + 3.65192E-03\text{Cp}^2 - 4.4091204E-06\text{Cp}^3 \\ & + 1.799033E-09\text{Cp}^4 \\ T(477.99) = & 102 \quad T(1124.68) = 596 \quad T(1329.02) = 994 \\ \text{std error est} = & 5.8 \quad \text{max error est} = 10 \end{aligned}$$

FLUOROMETHANE  $\text{CH}_3\text{F}$  200-1000K

$$\begin{aligned} \text{Cp}(T) = & 1472.3652 - 6.384875T + 0.0269437T^2 - 4.020256E-05T^3 \\ & + 2.816384E-08T^4 - 7.7050064E-12T^5 \\ \text{Cp}(200) = & 994.09 \quad \text{Cp}(600) = 1708.08 \quad \text{Cp}(1000) = 2289.27 \\ \text{std error est} = & 0.8 \quad \text{max error est} = 2.5 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) = & -2770.3792 + 6.5625134\text{Cp} - 5.26989E-03\text{Cp}^2 + 1.946297E-06\text{Cp}^3 \\ & - 2.543208E-10\text{Cp}^4 \\ T(994.09) = & 209 \quad T(1708.08) = 598 \quad T(2289.27) = 1000 \\ \text{std error est} = & 4.7 \quad \text{max error est} = 9.5 \end{aligned}$$

FORMALDEHYDE  $\text{HCHO}$  275-1500K

$$\begin{aligned} \text{Cp}(T) = & 1410.7255 - 3.85954T + 1.56866E-02T^2 - 2.25445E-05T^3 \\ & + 1.689E-08T^4 - 6.5741125E-12T^5 + 1.049515E-15T^6 \\ \text{Cp}(275) = & 1153.51 \quad \text{Cp}(800) = 1858.8 \quad \text{Cp}(1500) = 2366.67 \\ \text{std error est} = & 2.0 \quad \text{max error est} = 4.5 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) = & -302.25 - 0.79339952\text{Cp} + 2.386302E-03\text{Cp}^2 - 1.438642E-06\text{Cp}^3 \\ & + 2.990445E-10\text{Cp}^4 \\ T(1153.51) = & 279 \quad T(1858.8) = 798 \quad T(2366.67) = 1497 \\ \text{std error est} = & 3.9 \quad \text{max error est} = 7 \end{aligned}$$

FORMYL  $\text{HCO}$  300-1000K

$$\text{Cp}(T) = 978.65 + 0.6283T \quad T(\text{Cp}) = [\text{Cp} - 978.65]/0.6283$$

Note: There are only two data points in the reference source.

The accuracy of this fit cannot be adequately established.

FURAN  $\text{C}_4\text{H}_4\text{O}$  45-100K

$$\text{Cp}(T) = 1099.8 + 1.3061T \quad T(\text{Cp}) = [\text{Cp} - 1099.8]/1.3061$$

Note: There are only three data points in the reference source.

The accuracy of the fit cannot be adequately established.



HELIUM He ALL TEMPERATURES

Cp(T) = 519.31 - Constant - - - - -

n-HEPTANE - Ideal gas  $C_7H_{16}$  300-755K

$$Cp(T) = 94.626 + 5.860997T - 1.9823132E-03T^2 - 6.886993E-08T^3 - 1.9379526E-10T^4$$

$$Cp(300) = 1671.09 \quad Cp(500) = 2508.83 \quad Cp(755) = 3297.1$$

$$std\ error\ est = 0.2 \quad \quad \quad max\ error\ est = 1.0$$

755-1365K

$$Cp(T) = -740.308 + 10.893537T - 1.265124E-02T^2 + 9.843763E-06T^3 - 4.3228296E-09T^4 + 7.863665E-13T^5$$

$$Cp(755) = 3297.54 \quad Cp(1000) = 3809.29 \quad Cp(1365) = 4312.15$$

$$std\ error\ est = 0.3 \quad \quad \quad max\ error\ est = 1.0$$

300-755K

$$T(Cp) = -194.613 + 0.4265268Cp - 1.1575878E-04Cp^2 + 2.2332567E-08Cp^3$$

$$T(1671.09) = 299 \quad T(2508.83) = 500 \quad T(3297.1) = 754$$

$$std\ error\ est = 0.5 \quad \quad \quad max\ error\ est = 1.5$$

755-1365K

$$T(Cp) = -4882.496 + 4.4329699Cp - 1.260663E-03Cp^2 + 1.318505E-07Cp^3$$

$$T(3297.54) = 755 \quad T(3809.29) = 999 \quad T(4312.15) = 1364$$

std error est = 0.9 - - - - - max error est = 2.5

HEXAFLUOROETHANE  $(CF_3)_2$  175-1175K

$$Cp(T) = 659.43 - 2.9660847T + 2.168867E-02T^2 - 4.922597E-05T^3 + 5.4905868E-08T^4 - 3.068691E-11T^5 + 6.876342E-15T^6$$

$$Cp(175) = 587.42 \quad Cp(675) = 1148.43 \quad Cp(1175) = 1286.31$$

$$std\ error\ est = 4.9 \quad \quad \quad max\ error\ est = 11.0$$

n-HEXANE - Ideal gas  $C_6H_{14}$  275-755K

$$Cp(T) = 244.084 + 5.0862655T - 5.31415E-04T^2 - 1.0882839E-06T^3$$

$$Cp(275) = 1579.99 \quad Cp(500) = 2518.33 \quad Cp(755) = 3312.93$$

$$std\ error\ est = 0.2 \quad \quad \quad max\ error\ est = 1.0$$

755-1365K

$$Cp(T) = 4009.13 - 11.718687T + 0.0298761T^2 - 2.9593554E-05T^3 + 1.375164E-08T^4 - 2.4932142E-12T^5$$

$$Cp(755) = 3312.16 \quad Cp(1000) = 3831.41 \quad Cp(1365) = 4339.26$$

$$std\ error\ est = 0.7 \quad \quad \quad max\ error\ est = 2.0$$

275-755K

$$T(Cp) = -209.84 + 0.4334954Cp - 1.1488097E-04Cp^2 + 2.167164E-08Cp^3$$

$$T(1579.99) = 274 \quad T(2518.33) = 499 \quad T(3312.93) = 753$$

$$std\ error\ est = 0.6 \quad \quad \quad max\ error\ est = 2.5$$

755-1365K

$$T(Cp) = -5668.09 + 5.032992Cp - 1.41023E-03Cp^2 + 1.437634E-07Cp^3$$

$$T(3312.16) = 755 \quad T(3831.41) = 999 \quad T(4339.26) = 1364$$

n-HEXANE (continued)

std error est = 0.6 max error est = 2.5  
CYCLOHEXANE  $C_6H_{12}$  300-1500K

$$Cp(T) = -143.687 + 2.2338877T + 1.5757957E-02T^2 - 3.322767E-05T^3 \\ + 2.992193E-08T^4 - 1.3118055E-11T^5 + 2.278605E-15T^6$$

Cp(300) = 1259.7      Cp(800) = 3270.77      Cp(1500) = 4338.44  
std error est = 2.0      max error est = 3.5

300-1500K  
 $T(Cp) = 493.2108 - 0.6186162Cp + 5.38728E-04Cp^2 - 1.568782E-07Cp^3 \\ + 1.7939201E-11Cp^4$   
T(1259.7) = 300      T(3270.77) = 797      T(4338.44) = 1494  
std error est = 4.5 max error est = 10.0

HYDRAZINE  $N_2H_4$  275-1475K

$$Cp(T) = 164.415 + 6.9555374T - 7.864965E-03T^2 + 4.8061401E-06T^3 \\ - 1.14436786E-09T^4$$

Cp(275) = 1575.81      Cp(675) = 2516.48      Cp(1475) = 3319.06  
std error est = 4.3      max error est = 6.5

275-1475K  
 $T(Cp) = -382.0766 + 0.7822092Cp - 3.7974324E-04Cp^2 + 9.376375E-08Cp^3$   
T(1575.81) = 274      T(2516.48) = 676      T(3319.06) = 1459  
std error est = 7.5 max error est = 16.0

HYDROBROMIC ACID HBr 350-1500K

$$Cp(T) = 395.3995 - 0.2258915T + 4.5013067E-04T^2 - 2.807402E-07T^3 \\ + 6.0719708E-11T^4$$

Cp(350) = 360.35      Cp(850) = 387.9      Cp(1500) = 429.25  
std error est = 0.4      max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 350-1500K, Cp(T) =  $333.6168303 + 6.18710596E-02T + 2.6754517E-06T^2$ .

HYDROCYANIC ACID HCN 100-1500K

$$Cp(T) = 1044.92 - 0.430188124T + 9.2162939E-03T^2 - 2.1505599E-05T^3 \\ + 2.29172856E-08T^4 - 1.1686957E-11T^5 + 2.3027052E-15T^6$$

Cp(100) = 1074.74      Cp(800) = 1749.31      Cp(1500) = 2055.08  
std error est = 7.2      max error est = 16.5

100-1500K  
 $T(Cp) = -52339.698 + 171.0170866Cp - 0.2213524775Cp^2 + 1.4203695E-04Cp^3 \\ - 4.51189157E-08Cp^4 + 5.7079687E-12Cp^5$   
T(1074.74) = 95      T(1749.31) = 796      T(2055.08) = 1507  
std error est = 1.5 max error est = 7.5

HYDROFLUORIC ACID      HF                      100-1500K

$$\begin{aligned} \text{Cp}(T) = & 1460.773641 - 0.081301137T + 4.32324705E-04T^2 \\ & - 1.12701828E-06T^3 + 1.51594969E-09T^4 - 8.75540737E-13T^5 \\ & + 1.82375488E-16T^6 \end{aligned}$$

$$\begin{array}{lll} \text{Cp}(100) = 1455.98 & \text{Cp}(800) = 1477.23 & \text{Cp}(1500) = 1611.09 \\ \text{std error est} = 0.4 & & \text{max error est} = 1.0 \end{array}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K,  $\text{Cp}(T) = 1464.2305292 - 0.0715176125T + 1.1488975E-04T^2$ .

HYDROFLUORIC ACID,      DF                      300-1500K

MONODEUTERATED

$$\begin{aligned} \text{Cp}(T) = & 1317.953085 + 0.736930447T - 2.979053E-03T^2 + 5.585763E-06T^3 \\ & - 4.8632489E-09T^4 + 2.04262374E-12T^5 - 3.37598227E-16T^6 \end{aligned}$$

$$\begin{array}{lll} \text{Cp}(300) = 1387.06 & \text{Cp}(800) = 1449.66 & \text{Cp}(1500) = 1617.95 \\ \text{std error est} = 0.4 & & \text{max error est} = 1.5 \end{array}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 300-1500K,  $\text{Cp}(T) = 1444.09476 - 0.35547209T + 6.1254815E-04T^2 - 1.9925363E-07T^3$ .

HYDROGEN - Ideal gas      H<sub>2</sub>                      100-425K

$$\begin{aligned} \text{Cp}(T) = & 5006.6253 + 101.569422T - 0.602891517T^2 + 2.7375894E-03T^3 \\ & - 8.4758275E-06T^4 + 1.43800374E-08T^5 - 9.8072403E-12T^6 \end{aligned}$$

$$\begin{array}{lll} \text{Cp}(100) = 11158.65 & \text{Cp}(325) = 14334.47 & \text{Cp}(425) = 14498.83 \\ \text{std error est} = 3.2 & & \text{max error est} = 6.5 \end{array}$$

490-1365K

$$\begin{aligned} \text{Cp}(T) = & 14920.082 - 1.996917584T + 2.540615E-03T^2 - 4.7588954E-07T^3 \\ \text{Cp}(490) = 14495.61 & \text{Cp}(850) = 14766.04 & \text{Cp}(1365) = 15717.7 \\ \text{std error est} = 1.3 & & \text{max error est} = 4 \end{aligned}$$

Note: For temperatures between 425-490, Cp = 14494.7 - constant.

HYDROGEN - Real gas                      100-365K

$$\begin{aligned} \text{Cp}(T) = & 6436.5105 + 63.161307T - 0.1685728T^2 + 1.5229265E-04T^3 \\ \text{Cp}(100) = 11219.21 & \text{Cp}(225) = 13848.52 & \text{Cp}(365) = 14437.83 \\ \text{std error est} = 1.2 & & \text{max error est} = 2 \end{aligned}$$

365-475K

$$\begin{aligned} \text{Cp}(T) = & 29616.406 - 51.4939245T + 0.304123881T^2 - 4.2495904E-03T^3 \\ & + 1.9472701E-05T^4 - 3.55632306E-08T^5 + 2.30568584E-11T^6 \\ \text{Cp}(365) = 14440.87 & \text{Cp}(425) = 14506.73 & \text{Cp}(475) = 14512.49 \end{aligned}$$

HYDROGEN - Real gas (continued)

std error est = 2.0

max error est = 4.5

475-1255K

$$C_p(T) = 15009.352 - 2.2923455T + 2.869303E-03T^2 - 5.937169E-07T^3$$

$$C_p(475) = 14504.24 \quad C_p(875) = 14802.62 \quad C_p(1255) = 15478.11$$

std error est = 1.3

max error est = 5.5

HYDROGEN (Monatomic) H 100-1500K

Cp(T) = 20622 - constant

HYDROGEN, MONODEUTERATED HD 0-1500K

$$C_p(T) = 9648.403 + 0.180166208T - 4.410482E-04T^2 + 3.02156-1E-05T^3 \\ - 2.37468746E-09T^4 + 5.54340759E-13T^5$$

$$C_p(1) = 9648.58 \quad C_p(800) = 10266.28 \quad C_p(1500) = 11311.73$$

std error est = 0.6

max error est = 1.5

HYDROGEN CHLORIDE HCl 365-1365K

Ideal gas

$$C_p(T) = 770.99488 + 0.26534577T - 9.9858498E-04T^2 + 1.7010329E-06T^3 \\ - 1.1455977E-09T^4 + 2.736703E-13T^5$$

$$C_p(365) = 798.97 \quad C_p(850) = 843.13 \quad C_p(1365) = 918.63$$

std error est = 0.3

max error est = 1.0

Note: From 255-365K, Cp = 798.84 - constant.

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 365-1365K, Cp(T) =

$$841.8819 - 0.2461627T + 4.0609005E-04T^2 - 1.3558119E-07T^3$$

HYDROGEN IODIDE - Ideal gas HI 275-1365K

$$C_p(T) = 248.5266 - 0.15405244T + 3.53994265E-04T^2 - 2.5054778E-07T^3 \\ + 6.12525942E-11T^4$$

$$C_p(275) = 228.07 \quad C_p(875) = 252.82 \quad C_p(1365) = 273.24$$

std error est = 0.2

max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 275-1365K, Cp(T) =

$$214.2405 + 3.60151566E-02T + 6.81264406E-06T^2$$

HYDROGEN PEROXIDE H<sub>2</sub>O<sub>2</sub> 300-1500K

$$C_p(T) = 827.2894 + 1.66579757T - 6.5656617E-04T^2 + 4.920427E-08T^3$$

$$C_p(300) = 1269.27 \quad C_p(800) = 1764.92 \quad C_p(1500) = 2014.78$$

std error est = 0.6

max error est = 1.5

Note: For T(Cp) calculations, use the above equation and iteratives.

HYDROGEN SULFIDE - Ideal gas  $H_2S$  200-1365K

$$C_p(T) = 1001.424 - 0.442935517T + 2.03071482E-03T^2 - 1.946487E-06T^3 \\ + 8.5559054E-10T^4 - 1.51906275E-13T^5$$

$$C_p(200) = 979.81 \quad C_p(800) = 1250.81 \quad C_p(1365) = 1480.42$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.5$$

HYDROGEN SULFIDE,  $D_2S$  100-1500K

DIDEUTERATED

$$C_p(T) = 951.92162 - 0.636298T + 3.834902E-03T^2 - 5.1606288E-06T^3 \\ + 3.4347917E-09T^4 - 1.18396309E-12T^5 + 1.70442092E-16T^6$$

$$C_p(100) = 921.81 \quad C_p(800) = 1318.59 \quad C_p(1500) = 1548.24$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 1.5$$

100-1500K

$$T(C_p) = -164765.798 + 671.44529C_p - 1.09343063C_p^2 + 8.8987356E-04C_p^3 \\ - 3.61561554E-07C_p^4 + 5.87557715E-11C_p^5$$

$$T(921.81) = 129 \quad T(1318.59) = 803 \quad T(1548.24) = 1505$$

$$\text{std error est} = 8.5 \quad \text{max error est} = 29.0$$

HYDROGEN SULFIDE,  $T_2S$  50-250K

DITRITIATED

$$C_p(T) = 867.963 + 0.2747135T - 5.06698273E-03T^2 + 3.5644166E-05T^3 \\ - 6.07263928E-08T^4$$

$$C_p(50) = 873.08 \quad C_p(180) = 897.27 \quad C_p(250) = 939.54$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

Note: For  $T(C_p)$  calculations, use the iterative procedures discussed in Section 5 and the following eqn: 50-250K,  $C_p(T) =$

$$884.648608 - 0.326396624T + 2.20660346E-03T^2$$

HYDROGEN SULFIDE, HDS 50-1500K

MONODEUTERATED

$$C_p(T) = 962.62194 - 0.35271253T + 1.90644836E-03T^2 - 1.27551132E-06T^3 \\ - 3.3335115E-10T^4 + 6.2782923E-13T^5 - 1.75469178E-16T^6$$

$$C_p(50) = 949.59 \quad C_p(800) = 1270.71 \quad C_p(1500) = 1499.5$$

$$\text{std error est} = 1.3 \quad \text{max error est} = 2.5$$

HYDROGEN SULFIDE, MONO- DTS 100-250K

DEUTERATED/MONOTRITIATED

$$C_p(T) = 930.5966 - 0.671343T + 3.7680173E-03T^2 - 3.14889788E-06T^3$$

$$C_p(100) = 897.99 \quad C_p(175) = 911.63 \quad C_p(250) = 949.06$$

$$\text{std error est} = 0.3 \quad \text{max error est} = 1.5$$

100-250K

$$T(C_p) = -1873390.367 + 6052.319684C_p - 6.51827856C_p^2 + 2.3405097E-03C_p^3$$

$$T(897.99) = 109 \quad T(911.63) = 180 \quad T(949.09) = 257$$

$$\text{std error est} = 2.4 \quad \text{max error est} = 8.5$$

HYDROGEN SULFIDE, MONO- HTS 50-1500K

TRITIATED

$$Cp(T) = 947.2175 - 0.6001111T + 3.4256972E-03T^2 - 4.2387292E-06T^3 \\ + 2.28571453E-09T^4 - 4.6662046E-13T^5$$

$$Cp(50) = 925.26 \quad Cp(800) = 1272.67 \quad Cp(1500) = 1477.19$$

$$\text{std error est} = 2.2 \quad \text{max error est} = 6.5$$

HYDROXYL OH 0-1500K

$$Cp(T) = 1761.23799 - 0.2890543T + 7.1609328E-04T^2 - 3.6725166E-07T^3 \\ + 5.9334163E-11T^4$$

$$Cp(1) = 1760.95 \quad Cp(800) = 1824.56 \quad Cp(1500) = 1999.77$$

$$\text{std error est} = 3.0 \quad \text{max error est} = 5.5$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 0-1500K, Cp(T) =

$$1758.418762 - 0.236699T + 5.4753303E-04T^2 - 1.89130827E-07T^3$$

IODINE  $I_2$  250-1500K

$$Cp(T) = 131.03309 + 8.1451251E-02T - 1.4276222E-04T^2 + 1.088693E-07T^3 \\ - 2.9318658E-11T^4$$

$$Cp(250) = 144.06 \quad Cp(900) = 148.83 \quad Cp(1500) = 151.00$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.5$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, Cp(T) =

$$142.223033 + 1.13334775E-02T - 3.7835264E-06T^2$$

IODINE (Monatomic) 55-1550K

$$Cp(T) = 164.50 - \text{constant}$$

IODINE BROMIDE IBr 250-1500K

$$Cp(T) = 160.52687 + 8.1079813E-02T - 1.175744E-04T^2 + 7.647269E-08T^3 \\ - 1.81218914E-11T^4$$

$$Cp(250) = 174.57 \quad Cp(800) = 181.87 \quad Cp(1500) = 183.96$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, Cp(T) =

$$170.84732 + 2.05167565E-02T - 8.09243496E-06T^2$$

IODINE CHLORIDE ICl 250-1500K

$$Cp(T) = 186.45308 + 0.1656137T - 2.3408245E-04T^2 + 1.4813037E-07T^3 \\ - 3.44570338E-11T^4$$

IODINE CHLORIDE (continued)

Cp(250) = 215.41      Cp(800) = 230.86      Cp(1500) = 233.69  
std error est = 0.4      max error est = 1.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn; 250-1500K, Cp(T) =

$$207.56253 + 4.364782E-02T - 1.811719E-05T^2$$

IODINE FLUORIDE      IF      250-1500K

$$Cp(T) = 175.3521 + 0.26519153T - 3.3997426E-04T^2 + 1.9855293E-07T^3 - 4.316987E-11T^4$$

Cp(250) = 223.34      Cp(800) = 253.9      Cp(1500) = 259.77  
std error est = 0.4      max error est = 1.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn; 250-1500K, Cp(T) =

$$188.3318389 + 0.1798053T - 1.5965353E-04T^2 + 4.7953466E-08T^3$$

IODINE HEPTAFLUORIDE      IF<sub>7</sub>      250-1000K

$$Cp(T) = -386.25397 + 6.988192T - 2.19E-02T^2 + 3.9399594E-05T^3 - 4.11419754E-08T^4 + 2.31307177E-11T^5 - 5.40722595E-15T^6$$

Cp(250) = 468.22      Cp(600) = 647.34      Cp(1000) = 683.05  
std error est = 0.5      max error est = 1.5

IODINE PENTAFLUORIDE      IF<sub>5</sub>      250-1500K

$$Cp(T) = -58.2197 + 3.228146T - 7.466701E-03T^2 + 9.66136789E-06T^3 - 7.133844E-09T^4 + 2.80488185E-12T^5 - 4.551596E-16T^6$$

Cp(250) = 407.87      Cp(800) = 569.99      Cp(1500) = 590.97  
std error est = 0.5      max error est = 1.5

IODOMETHANE      CH<sub>3</sub>I      300-600K

$$Cp(T) = 238.1717 \exp(0.0011T) \quad \text{max error est} = 5.0\%$$

ISOPRENE      CH<sub>2</sub>C(CH<sub>3</sub>)CHCH<sub>2</sub>      275-1500K

$$Cp(T) = -396.2635 + 8.948094T - 1.0120624E-02T^2 + 7.068983E-06T^3 - 2.65012106E-09T^4 + 3.98613124E-13T^5$$

Cp(275) = 1431.57      Cp(900) = 3109.24      Cp(1500) = 3723.02  
std error est = 1.9      max error est = 4.5

275-1500K

$$T(Cp) = 1061.69 - 1.77172Cp + 1.3189685E-03Cp^2 - 3.9005614E-07Cp^3 + 4.618566E-11Cp^4$$

T(1431.57) = 278      T(3109.24) = 896      T(3723.02) = 1492  
std error est = 4.4      max error est = 8.5

KETENE       $\text{H}_2\text{CCO}$       250-1500K

$$\begin{aligned}\text{Cp}(T) &= 399.1048 + 2.617846T + 5.971587\text{E-}04T^2 - 5.279979\text{E-}06T^3 \\ &\quad + 6.195382\text{E-}09T^4 - 3.1370787\text{E-}12T^5 + 6.0082048\text{E-}16T^6 \\ \text{Cp}(250) &= 1029.67 & \text{Cp}(800) &= 1839.39 & \text{Cp}(1500) &= 2235.20 \\ \text{std error est} &= 1.0 & & & \text{max error est} &= 2.5\end{aligned}$$

250-1500K

$$\begin{aligned}\text{T}(\text{Cp}) &= 2213.102 - 6.36729113\text{Cp} + 7.14666\text{E-}03\text{Cp}^2 - 3.3641974\text{E-}06\text{Cp}^3 \\ &\quad + 6.1602663\text{E-}10\text{Cp}^4\end{aligned}$$

$$\text{T}(1029.67) = 254 \quad \text{T}(1839.39) = 796 \quad \text{T}(2235.20) = 1494$$

$$\text{std error est} = 4.0 \quad \text{max error est} = 8.5$$

KRYPTON      Kr      ALL TEMPERATURES

$$\text{Cp}(T) = 248.05 - \text{constant}$$

MESITYLENE       $\text{C}_6\text{H}_3(\text{CH}_3)_3$       300-1500K

$$\begin{aligned}\text{Cp}(T) &= 240.097 + 2.177066T + 7.26309147\text{E-}03T^2 - 1.36166\text{E-}05T^3 \\ &\quad + 9.1161133\text{E-}09T^4 - 2.1807381\text{E-}12T^5 \\ \text{Cp}(300) &= 1247.79 & \text{Cp}(800) &= 2677.81 & \text{Cp}(1500) &= 3481.97 \\ \text{std error est} &= 1.5 & & & \text{max error est} &= 2.5\end{aligned}$$

300-1500K

$$\begin{aligned}\text{T}(\text{Cp}) &= 439.7914 - 0.759142\text{Cp} + 8.223984\text{E-}04\text{Cp}^2 - 2.963892\text{E-}07\text{Cp}^3 \\ &\quad + 4.24823947\text{E-}11\text{Cp}^4\end{aligned}$$

$$\text{T}(1247.79) = 300 \quad \text{T}(2677.81) = 797 \quad \text{T}(3481.97) = 1500$$

$$\text{std error est} = 2.9 \quad \text{max error est} = 4.5$$

METHANE - Ideal gas       $\text{CH}_4$       275-755K

$$\begin{aligned}\text{Cp}(T) &= 1916.5258 - 1.09269T + 8.696605\text{E-}03T^2 - 5.2291144\text{E-}06T^3 \\ \text{Cp}(275) &= 2164.97 & \text{Cp}(500) &= 2890.69 & \text{Cp}(755) &= 3799.38 \\ \text{std error est} &= 0.2 & & & \text{max error est} &= 1.0\end{aligned}$$

755-1365K

$$\begin{aligned}\text{Cp}(T) &= 10435.6 - 42.025284T + 8.849006\text{E-}02T^2 - 8.4304566\text{E-}05T^3 \\ &\quad + 3.9030203\text{E-}08T^4 - 7.1345169\text{E-}12T^5\end{aligned}$$

$$\text{Cp}(755) = 3797.77 \quad \text{Cp}(1000) = 4491.5 \quad \text{Cp}(1365) = 5224.89$$

$$\text{std error est} = 1.0 \quad \text{max error est} = 2.5$$

275-755K

$$\begin{aligned}\text{T}(\text{Cp}) &= -1405.54 + 1.36736\text{Cp} - 3.55452\text{E-}04\text{Cp}^2 + 3.823585\text{E-}08\text{Cp}^3 \\ \text{T}(2164.97) &= 277 & \text{T}(2890.69) &= 500 & \text{T}(3799.38) &= 756\end{aligned}$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 2.5$$

755-1365K

$$\begin{aligned}\text{T}(\text{Cp}) &= -2892.182 + 2.2452\text{Cp} - 5.10113\text{E-}04\text{Cp}^2 + 4.52369\text{E-}08\text{Cp}^3 \\ \text{T}(3797.77) &= 755 & \text{T}(4491.5) &= 1000 & \text{T}(5224.89) &= 1365\end{aligned}$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 2.5$$

METHANE - Real gas



METHANE - Real gas (continued) 275-510K

$$\begin{aligned} \text{Cp}(T) &= -12236.8831 + 262.518875T - 1.9826045T^2 + 7.840392E-03T^3 \\ &\quad - 1.70541464E-05T^4 + 1.9431809E-08T^5 - 9.08114724E-12T^6 \\ \text{Cp}(275) &= 2175.89 \quad \text{Cp}(375) = 2457.67 \quad \text{Cp}(510) = 2912.87 \\ \text{std error est} &= 2.7 \quad \text{max error est} = 6.5 \end{aligned}$$

275-510K

$$\begin{aligned} T(\text{Cp}) &= -742.678 + 0.58853377\text{Cp} - 5.46177054E-05\text{Cp}^2 \\ T(2175.89) &= 279 \quad T(2457.67) = 374 \quad T(2912.87) = 508 \\ \text{std error est} &= 2.8 \quad \text{max error est} = 5.5 \end{aligned}$$

METHANE, DIDEUTERATED  $\text{CH}_2\text{D}_2$  95-1275K

$$\begin{aligned} \ln[\text{Cp}(T)] &= 7.6070340658 - 1.74744883E-03T + 9.23134494E-06T^2 \\ &\quad - 1.06684914E-08T^3 + 3.85790574E-12T^4 \\ \text{Cp}(95) &= 1836.3 \quad \text{Cp}(675) = 3475.02 \quad \text{Cp}(1275) = 4762.75 \\ \text{**Note: Cp}(T) &= \exp[\text{fctn}(T)] \quad \text{max error est} = 45.0 \end{aligned}$$

METHANE, DIDEUTERATED  $\text{CD}_2\text{T}_2$  95-1275K

$$\begin{aligned} \text{DITRITIATED} \\ \text{Cp}(T) &= 1858.141 - 6.9817888T + 4.033067E-02T^2 - 6.835852E-05T^3 \\ &\quad + 5.20572E-08T^4 - 1.490558E-11T^5 \\ \text{Cp}(95) &= 1504.37 \quad \text{Cp}(675) = 3215.76 \quad \text{Cp}(1275) = 4180.76 \\ \text{std error est} &= 3.0 \quad \text{max error est} = 6.5 \end{aligned}$$

METHANE, DITRITIATED  $\text{CH}_2\text{T}_2$  95-1275K

$$\begin{aligned} \text{Cp}(T) &= 1861.969 - 3.8411072T + 1.9495867E-02T^2 - 2.0658472E-05T^3 \\ &\quad + 7.0155845E-09T^4 \\ \text{Cp}(95) &= 1655.87 \quad \text{Cp}(675) = 3254.97 \quad \text{Cp}(1275) = 4379.07 \\ \text{std error est} &= 7.2 \quad \text{max error est} = 15.0 \end{aligned}$$

METHANE, MONODEUTERATED  $\text{CH}_3\text{D}$  95-1275K

$$\begin{aligned} \ln[\text{Cp}(T)] &= 7.685260605 - 1.89630346E-03T + 8.85273067E-06T^2 \\ &\quad - 9.69191539E-09T^3 + 3.378275E-12T^4 \\ \text{Cp}(95) &= 1952.7 \quad \text{Cp}(675) = 3495.99 \quad \text{Cp}(1275) = 4905.71 \\ \text{**Note: Cp}(T) &= \exp[\text{fctn}(T)] \quad \text{max error est} = 9.5 \end{aligned}$$

METHANE, MONODEUTERATED,  $\text{CDT}_3$  95-1275K

$$\begin{aligned} \text{TRITRITIATED} \\ \text{Cp}(T) &= 1792.8646 - 7.153158T + 4.2595806E-02T^2 - 7.46524585E-05T^3 \\ &\quad + 5.84466516E-08T^4 - 1.70935846E-11T^5 \\ \text{Cp}(95) &= 1438.36 \quad \text{Cp}(675) = 3150.99 \quad \text{Cp}(1275) = 4046.87 \\ \text{std error est} &= 1.2 \quad \text{max error est} = 2.5 \end{aligned}$$

METHANE, MONOTRITIATED  $\text{CH}_3\text{T}$  95-1275K

$$\begin{aligned} \ln[\text{Cp}(T)] &= 7.623967385 - 1.89530858E-03T + 9.19540139E-06T^2 \\ &\quad - 1.02844644E-08T^3 + 3.63747258E-12T^4 \end{aligned}$$

METHANE, MONOTRITIATED (continued)

Cp(95) = 1841.58 Cp(675) = 3382.78 Cp(1275) = 4684.41  
 \*\*Note: Cp(T) = exp[fctn(T)] max error est = 11.5

METHANE, TETRADEUTERATED CD<sub>4</sub> 95-1275K

ln[Cp(T)] = 7.6175941054 - 4.03359764E-03T + 2.34289511E-05T<sup>2</sup>  
 - 4.27574857E-08T<sup>3</sup> + 3.43557214E-11T<sup>4</sup> - 1.01858966E-14T<sup>5</sup>  
 Cp(95) = 1655.58 Cp(675) = 3376.31 Cp(1275) = 4488.86  
 \*\*Note: Cp(T) = exp[fctn(T)] max error est = 15.0

METHANE, TETRATRITIATED CT<sub>4</sub> 95-1275K

Cp(T) = 1736.415 - 7.3850897T + 4.525255E-02T<sup>2</sup> - 8.1987002E-05T<sup>3</sup>  
 + 6.5925034E-08T<sup>4</sup> - 1.9662464E-11T<sup>5</sup>  
 Cp(95) = 1378.16 Cp(675) = 3085.25 Cp(1275) = 3918.72  
 std error est = 2.9 max error est = 9.5

METHANE, TRIDEUTERATED CHD<sub>3</sub> 95-1275K

Cp(T) = 1967.71 - 4.14269394T + 2.0693509E-02T<sup>2</sup> - 2.1823919E-05T<sup>3</sup>  
 + 7.39241354E-09T<sup>4</sup>  
 Cp(95) = 1742.80 Cp(675) = 3422.62 Cp(1275) = 4627.45  
 std error est = 8.8 max error est = 15.0

METHANE, TRIDEUTERATED, CD<sub>3</sub>T 95-1275K

MONOTRITIATED

Cp(T) = 1909.6275 - 6.445028T + 3.602721E-02T<sup>2</sup> - 5.7366078E-05T<sup>3</sup>  
 + 4.11246853E-08T<sup>4</sup> - 1.11879465E-11T<sup>5</sup>  
 Cp(95) = 1576.57 Cp(675) = 3300.89 Cp(1275) = 4339.79  
 std error est = 5.3 max error est = 11.0

METHANE, TRITRITIATED CHT<sub>3</sub> 95-1275K

Cp(T) = 1793.405 - 5.700601T + 3.260151E-02T<sup>2</sup> - 5.1462346E-05T<sup>3</sup>  
 + 3.64062843E-08T<sup>4</sup> - 9.77635312E-12T<sup>5</sup>  
 Cp(95) = 1504.84 Cp(675) = 3160.29 Cp(1275) = 4127.4  
 std error est = 3.6 max error est = 6.5

METHANETHIOL CH<sub>3</sub>SH 300-1000K

Cp(T) = 706.9902 + 0.0461346T + 6.2988574E-03T<sup>2</sup> - 1.0655555E-05T<sup>3</sup>  
 + 7.67648136E-09T<sup>4</sup> - 2.11193895E-12T<sup>5</sup>

Cp(300) = 1057.08 Cp(700) = 1659.04 Cp(1000) = 1960.97  
 std error est = 0.5 max error est = 2.5

300-1000K

T(Cp) = -689.19 + 1.5805785Cp - 8.9447465E-04Cp<sup>2</sup> + 2.6908387E-07Cp<sup>3</sup>  
 T(1057.08) = 300 T(1659.04) = 700 T(1960.97) = 1000

std error est = 0.4 max error est = 1.5

METHYL CH<sub>3</sub> 300-1000K

$$C_p(T) = 1633.77 + 2.1942T \quad T(C_p) = [C_p - 1633.77]/2.1942$$

Note: There are only two data points in the reference source.

The accuracy of the fit cannot be adequately established.

METHYL ACETATE CH<sub>3</sub>COOCH<sub>3</sub> 410K

Cp = 1540 - constant

Note: There is but a single data point in the reference source.

METHYL ALCOHOL CH<sub>3</sub>OH 275-975K

Ideal gas

$$C_p(T) = 468.2325 + 5.233369T - 1.468378E-02T^2 + 3.72060479E-05T^3 \\ - 4.766607E-08T^4 + 2.879509E-11T^5 - 6.5351158E-15T^6$$

$$C_p(275) = 1340.57 \quad C_p(675) = 2274.68 \quad C_p(975) = 2778.64 \\ \text{std error est} = 0.6 \quad \text{max error est} = 2.0$$

275-975K

$$T(C_p) = -704.043 + 1.17817452C_p - 4.5448512E-04C_p^2 + 8.93023618E-08C_p^3$$

$$T(1340.57) = 274 \quad T(2274.68) = 675 \quad T(2778.64) = 977$$

$$\text{std error est} = 0.8 \quad \text{max error est} = 2.5$$

METHYLAMINE CH<sub>3</sub>NH<sub>2</sub> 275-1475K

$$C_p(T) = 943.047 + 0.1489865T + 1.356349E-02T^2 - 2.595927E-05T^3 \\ + 2.34257414E-08T^4 - 1.05893911E-11T^5 + 1.91432176E-15T^6$$

$$C_p(275) = 1588.03 \quad C_p(875) = 3226.76 \quad C_p(1475) = 4031.33 \\ \text{std error est} = 2.0 \quad \text{max error est} = 4.5$$

275-1475K

$$T(C_p) = 417.62 - 0.72820643C_p + 6.4038758E-04C_p^2 - 1.8338439E-07C_p^3 \\ + 2.11959172E-11C_p^4$$

$$T(1588.03) = 277 \quad T(3226.76) = 872 \quad T(4031.33) = 1473$$

$$\text{std error est} = 2.3 \quad \text{max error est} = 4.5$$

2-METHYLBUTANE (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> 300-1500K

$$C_p(T) = 153.06 + 4.3328259T + 6.6922173E-03T^2 - 1.8629145E-05T^3 \\ + 1.81902873E-08T^4 - 8.3598691E-12T^5 + 1.4996865E-15T^6$$

$$C_p(300) = 1680.34 \quad C_p(800) = 3468.73 \quad C_p(1500) = 4524.36 \\ \text{std error est} = 1.6 \quad \text{max error est} = 4.0$$

300-1500K

$$T(C_p) = 732.49 - 1.00072568C_p + 6.833615E-04C_p^2 - 1.725454E-07C_p^3 \\ + 1.73798873E-11C_p^4$$

$$T(1680.34) = 300 \quad T(3468.73) = 798 \quad T(4524.36) = 1496$$

$$\text{std error est} = 3.4 \quad \text{max error est} = 7.5$$

2-METHYL-2-BUTANOL  $(\text{CH}_3)_2\text{COHCH}_2\text{CH}_3$  400-575K

$$\ln[\text{Cp}(T)] = 722.5726607 - 5.769804449T + 0.012524666T^2 \\ + 1.60592914E-05T^3 - 1.06765564E-07T^4 + 1.57879296E-10T^5 \\ - 7.86807765E-14T^6$$

$$\text{Cp}(400) = 2000.65 \quad \text{Cp}(500) = 2301.88 \quad \text{Cp}(575) = 2736.30$$

- **\*\*Note:**  $\text{Cp}(T) = \exp[\text{fctn}(T)]$  - - - - - max error est = 10.0

3-METHYL-1-BUTANOL  $(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{OH}$  450-500K

$$\text{Cp}(T) = 12449.8133 - 46.47211274T + 5.25188485E-02T^2$$

$$\text{Cp}(450) = 2172.43 \quad \text{Cp}(475) = 2225.12 \quad \text{Cp}(500) = 2343.47 \\ \text{std error est} = 1.1 \quad \text{max error est} = 4.5$$

450-500K

$$T(\text{Cp}) = -6275.55 + 5.7093249\text{Cp} - 1.20269088E-03\text{Cp}^2$$

$$T(2172.43) = 452 \quad T(2225.12) = 474 \quad T(2343.47) = 499$$

- std error est = 2.4 - - - - - max error est = 6.0

3-METHYL-1-BUTYNE  $(\text{CH}_3)_2\text{CHCCH}$  300-1500K

$$\text{Cp}(T) = 17.777 + 6.352748T - 4.78347376E-03T^2 + 1.9843222E-06T^3 \\ - 3.49882302E-10T^4$$

$$\text{Cp}(300) = 1543.83 \quad \text{Cp}(800) = 2911.21 \quad \text{Cp}(1500) = 3709.89 \\ \text{std error est} = 2.0 \quad \text{max error est} = 4.5$$

300-1500K

$$T(\text{Cp}) = 1134.29 - 1.94512287\text{Cp} + 1.4522943E-03\text{Cp}^2 - 4.2842051E-07\text{Cp}^3 \\ + 4.99658252E-11\text{Cp}^4$$

$$T(1543.83) = 300 \quad T(2911.21) = 799 \quad T(3709.89) = 1496$$

- std error est = 2.9 - - - - - max error est = 6.5

METHYL CHLORIDE  $\text{CH}_3\text{Cl}$  255-755K

Ideal gas

$$\text{Cp}(T) = 332.8997 + 1.6366402T - 3.801244E-05T^2 - 4.04253913E-07T^3$$

$$\text{Cp}(275) = 771.69 \quad \text{Cp}(500) = 1091.19 \quad \text{Cp}(755) = 1372.92 \\ \text{std error est} = 0.2 \quad \text{max error est} = 2.5$$

755-1365K

$$\text{Cp}(T) = 526.238 + 1.16955813T + 2.7488708E-04T^2 - 5.75072686E-07T^3 \\ + 1.67250614E-10T^4$$

$$\text{Cp}(755) = 1372.8 \quad \text{Cp}(1000) = 1562.86 \quad \text{Cp}(1365) = 1752.91 \\ \text{std error est} = 0.1 \quad \text{max error est} = 1.0$$

255-755K

$$T(\text{Cp}) = -458.583 + 1.4667588\text{Cp} - 9.82376432E-04\text{Cp}^2 + 4.05810172E-07\text{Cp}^3$$

$$T(771.69) = 275 \quad T(1091.19) = 499 \quad T(1372.92) = 754 \\ \text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

755-1365K

$$T(\text{Cp}) = -6942.55 + 14.831976\text{Cp} - 1.0193339E-02\text{Cp}^2 + 2.5303315E-06\text{Cp}^3$$

$$T(1372.8) = 755 \quad T(1562.86) = 999 \quad T(1752.91) = 1364 \\ \text{std error est} = 0.6 \quad \text{max error est} = 1.5$$

METHYL CYANIDE  $\text{CH}_3\text{CN}$  290-1200K

$$\text{Cp}(T) = 1303.384 - 4.942871T + 2.849223E-02T^2 - 5.4871983E-05T^3 \\ + 5.3623977E-08T^4 - 2.63165765E-11T^5 + 5.11566313E-15T^6$$

$\text{Cp}(290) = 1256.21$        $\text{Cp}(650) = 1963.81$        $\text{Cp}(1200) = 2567.87$   
 std error est = 1.7      max error est = 4.5

290-1200K

$$T(\text{Cp}) = -813.42 + 1.58371\text{Cp} - 8.002791E-04\text{Cp}^2 + 1.8985947E-07\text{Cp}^3$$

$T(1256.21) = 290$        $T(1963.81) = 648$        $T(2567.87) = 1192$   
 \_ std error est = 4.4 \_ \_ \_ \_ \_ max error est = 9.5 \_

METHYL ETHER  $(\text{CH}_3)_2\text{O}$  275-1275K

$$\text{Cp}(T) = 626.107 + 2.175166T + 2.77749E-03T^2 - 3.7041748E-06T^3 \\ + 1.1994434E-09T^4$$

$\text{Cp}(275) = 1364.15$        $\text{Cp}(675) = 2469.63$        $\text{Cp}(1275) = 3406.78$   
 std error est = 7.2      max error est = 15.5

275-1275K

$$T(\text{Cp}) = -687.49 + 1.161406\text{Cp} - 4.4639784E-04\text{Cp}^2 + 8.05362496E-08\text{Cp}^3$$

$T(1364.15) = 271$        $T(2469.63) = 671$        $T(3406.78) = 1273$   
 \_ std error est = 6.3 \_ \_ \_ \_ \_ max error est = 10.5 \_

METHYLHYDRAZINE  $\text{CH}_3\text{NHNH}_2$  300-1500K

$$\text{Cp}(T) = -230.3353 + 8.3735806T - 1.038813E-02T^2 + 8.570289E-06T^3 \\ - 3.9110406E-09T^4 + 7.27987797E-13T^5$$

$\text{Cp}(300) = 1548.29$        $\text{Cp}(800) = 2844.7$        $\text{Cp}(1500) = 3609.98$   
 std error est = 5.1      max error est = 10.5

300-1500K

$$T(\text{Cp}) = 1646.485 - 2.833585\text{Cp} + 2.0125928E-03\text{Cp}^2 - 5.8370013E-07\text{Cp}^3 \\ + 6.66115245E-11\text{Cp}^4$$

$T(1548.29) = 300$        $T(2844.7) = 798$        $T(3609.98) = 1498$   
 \_ std error est = 4.7 \_ \_ \_ \_ \_ max error est = 7.5 \_

METHYLIDYNE  $\text{CH}$  300-1000K

$$\text{Cp}(T) = 2156.83 + 0.2622T \quad T(\text{Cp}) = [\text{Cp} - 2156.83]/0.2622$$

Note: There are only two data points in the reference source.

\_ The accuracy of the fit cannot be adequately established. \_ \_ \_ \_ \_

METHYL ISOCYANIDE  $\text{CH}_3\text{NC}$  275-755K

$$\text{Cp}(T) = 357.656 + 6.2401786T - 2.013433E-02T^2 + 4.623548E-05T^3 \\ - 5.0729918E-08T^4 + 2.0834756E-11T^5$$

$\text{Cp}(275) = 1255.24$        $\text{Cp}(500) = 1704.06$        $\text{Cp}(755) = 2117.84$   
 std error est = 1.7      max error est = 20.0

METHYL ISOCYANIDE (continued) 275-755K

$$T(Cp) = -929.29 + 1.6998Cp - 8.2667574E-04Cp^2 + 1.88543E-07Cp^3$$

$$T(1255.24) = 275 \quad Cp(1704.06) = 500 \quad Cp(2117.84) = 754$$

$$\text{std error est} = 0.9 \quad \text{max error est} = 3.5$$

2-METHYLPENTANE  $(CH_3)_2CH(CH_2)_2CH_3$  300-1000K

$$Cp(T) = 684.245 - 5.70106E-03T + 1.9830116E-02T^2 - 3.690549E-05T^3$$

$$+ 2.8436028E-08T^4 - 8.1932667E-12T^5$$

$$Cp(300) = 1681.22 \quad Cp(600) = 2896.28 \quad Cp(1000) = 3845.93$$

$$\text{std error est} = 2.0 \quad \text{max error est} = 4.5$$

300-1000K

$$T(Cp) = -220.405 + 0.475071Cp - 1.430724E-04Cp^2 + 2.652954E-08Cp^3$$

$$T(1681.22) = 300 \quad T(2896.28) = 600 \quad T(3845.93) = 1000$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 2.5$$

3-METHYLPENTANE  $[CH_3CH_2]_2CH(CH_3)$  300-1000K

$$Cp(T) = 1424.458 - 8.421426T + 6.009702E-02T^2 - 1.35448706E-04T^3$$

$$+ 1.5779472E-07T^4 - 9.48522387E-11T^5 + 2.3256203E-14T^6$$

$$Cp(300) = 1714.25 \quad Cp(600) = 2909.14 \quad Cp(1000) = 3850.03$$

$$\text{std error est} = 1.4 \quad \text{max error est} = 3.5$$

300-1000K

$$T(Cp) = -226.975 + 0.4721466Cp - 1.4127356E-04Cp^2 + 2.633499E-08Cp^3$$

$$T(1714.25) = 300 \quad T(2909.14) = 599 \quad T(3850.03) = 1000$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 2.5$$

4-METHYL-2-PENTANONE  $CH_3COCH_2CH(CH_3)_2$  275-1275K

$$Cp(T) = 266.655 + 4.794024T - 2.2291946E-03T^2 + 3.4395827E-07T^3$$

$$Cp(275) = 1423.58 \quad Cp(675) = 2592.73 \quad Cp(1275) = 3468.11$$

$$\text{std error est} = 7.0 \quad \text{max error est} = 15.5$$

275-1275K

$$T(Cp) = 892.053 - 1.68075Cp + 1.3909914E-03Cp^2 - 4.3712435E-07Cp^3$$

$$+ 5.3282889E-11Cp^4$$

$$T(1423.58) = 276 \quad T(2592.73) = 674 \quad T(3468.11) = 1268$$

$$\text{std error est} = 8.1 \quad \text{max error est} = 17.5$$

2-METHYL-1-PROPANOL  $(CH_3)_2CHCH_2OH$  390-600K

$$Cp(T) = 66430.768 - 523.644673T + 1.572952115T^2 - 2.07471664E-03T^3$$

$$+ 1.01994038E-06T^4$$

$$Cp(390) = 1980.96 \quad Cp(500) = 2253.15 \quad Cp(600) = 2552.20$$

$$\text{std error est} = 8.1 \quad \text{max error est} = 15.5$$

390-600K

$$T(Cp) = -585.026 + 0.6296626Cp - 6.49129487E-05Cp^2$$

$$T(1980.96) = 407 \quad T(2253.15) = 504 \quad T(2552.20) = 599$$

$$\text{std error est} = 7.9 \quad \text{max error est} = 17.5$$

2-METHYL-2-PROPANOL (CH<sub>3</sub>)<sub>3</sub>COH 360-590K

$$\begin{aligned} \text{Cp}(T) &= 1159558.4 - 14251.01382T + 72.825463058T^2 - 0.1978064T^3 \\ &\quad + 3.0125819E-04T^4 - 2.4393359E-07T^5 + 8.2046497E-11T^6 \\ \text{Cp}(360) &= 2123.03 \quad \text{Cp}(450) = 2152.98 \quad \text{Cp}(590) = 2625.67 \\ \text{std error est} &= 3.9 \quad \text{max error est} = 10.5 \end{aligned}$$

2-METHYLPROPENE (CH<sub>3</sub>)<sub>2</sub>CCH<sub>2</sub> 275-1500K

$$\begin{aligned} \text{Cp}(T) &= 360.3445 + 3.60460787T + 4.45078E-03T^2 - 1.2087027E-05T^3 \\ &\quad + 1.1350898E-08T^4 - 5.08523225E-12T^5 + 8.992065E-16T^6 \\ \text{Cp}(275) &= 1494.14 \quad \text{Cp}(800) = 3122.69 \quad \text{Cp}(1500) = 4078.26 \\ \text{std error est} &= 1.1 \quad \text{max error est} = 8.0 \end{aligned}$$

$$\begin{aligned} T(\text{Cp}) &= 675.5 - 1.08191523\text{Cp} + 8.400338E-04\text{Cp}^2 - 2.3638415E-07\text{Cp}^3 \\ &\quad + 2.637218E-11\text{Cp}^4 \\ T(1494.14) &= 277 \quad T(3122.69) = 798 \quad T(4078.26) = 1496 \\ \text{std error est} &= 2.8 \quad \text{max error est} = 5.5 \end{aligned}$$

METHYL SULFIDE (CH<sub>3</sub>)<sub>2</sub>S 300-1000K

$$\begin{aligned} \text{Cp}(T) &= -275.0796 + 10.650717T - 3.669097E-02T^2 + 8.1787615E-05T^3 \\ &\quad - 9.94226515E-08T^4 + 6.1455998E-11T^5 - 1.51906388E-14T^6 \\ \text{Cp}(300) &= 1159.15 \quad \text{Cp}(600) = 1757.63 \quad \text{Cp}(1000) = 2314.99 \\ \text{std error est} &= 0.7 \quad \text{max error est} = 2.5 \\ T(\text{Cp}) &= -553.78 + 1.1759729\text{Cp} - 5.4085555E-04\text{Cp}^2 + 1.3944132E-07\text{Cp}^3 \\ T(1159.15) &= 300 \quad T(1757.63) = 599 \quad T(2314.99) = 1000 \\ \text{std error est} &= 1.0 \quad \text{max error est} = 2.5 \end{aligned}$$

NEON Ne Ideal gas ALL TEMPERATURES

$$\text{Cp}(T) = 1029.91 - \text{constant}$$

NITRIC OXIDE - Ideal gas NO 110-1365K

$$\begin{aligned} \text{Cp}(T) &= 1188.304 - 1.4425597T + 3.465558E-03T^2 - 2.861451E-06T^3 \\ &\quad + 4.0387214E-10T^4 + 6.1972525E-13T^5 - 2.4090578E-16T^6 \\ \text{Cp}(110) &= 1067.82 \quad \text{Cp}(800) = 1092.5 \quad \text{Cp}(1365) = 1179.32 \\ \text{std error est} &= 0.3 \quad \text{max error est} = 2.5 \end{aligned}$$

NITRIC OXIDE - Real gas 165-645K

$$\begin{aligned} \text{Cp}(T) &= 1378.8188 - 3.82241T + 1.7887256E-02T^2 - 5.6028657E-05T^3 \\ &\quad + 1.16489E-07T^4 - 1.32980437E-10T^5 + 6.13527678E-14T^6 \\ \text{Cp}(165) &= 1054.73 \quad \text{Cp}(400) = 997.68 \quad \text{Cp}(645) = 1054.39 \\ \text{std error est} &= 0.3 \quad \text{max error est} = 1.5 \end{aligned}$$

NITRIC OXIDE - Real gas (continued) 645-1365K

$$C_p(T) = 806.451 + 0.506398T - 2.0853977E-04T^2 + 2.8257004E-08T^3$$

Cp(645) = 1053.90      Cp(1000) = 1132.57      Cp(1365) = 1180.99  
std error est = 0.2      max error est = 1.5

$$T(C_p) = -152350.55 + 425.34707C_p - 0.39764893C_p^2 + 1.2506075E-04C_p^3$$

T(1053.90) = 645      T(1132.57) = 998      T(1180.99) = 1361  
std error est = 2.0      max error est = 4.5

NITROGEN - Ideal gas  $N_2$  255-590K

$$C_p(T) = 1088.047 - 0.355968T + 7.2907605E-04T^2 - 2.8861556E-07T^3$$

Cp(255) = 1039.9      Cp(450) = 1049.2      Cp(590) = 1072.54  
std error est = 0.1      max error est = 1.0

$$C_p(T) = 1405.5077 - 2.1894566T + 4.7852898E-03T^2 - 4.540166E-06T^3$$

$$+ 2.08491259E-09T^4 - 3.7903033E-13T^5$$

Cp(590) = 1072.57      Cp(1000) = 1167.06      Cp(1365) = 1227.83  
std error est = 0.1      max error est = 1.5

Note: For T(Cp) calculations from 255-590K, use the iterative procedures discussed in Section 5 and the following eqn: 255-590K,  
 $C_p(T) = 1068.513739 - 0.20687009T + 3.63655082E-04T^2$ .

$$T(C_p) = -126050.925 + 333.06633C_p - 0.295083212C_p^2 + 8.823403E-05C_p^3$$

T(1072.57) = 592      T(1167.06) = 1000      T(1227.83) = 1365  
std error est = 0.8      max error est = 4.5

NITROGEN - Real gas 255-1365K

$$C_p(T) = 1058.5365 - 4.391145E-03T - 7.6852515E-04T^2 + 2.751091E-06T^3$$

$$- 3.1245817E-09T^4 + 1.5407594E-12T^5 - 2.8488096E-16T^6$$

Cp(255) = 1041.43      Cp(800) = 1122.09      Cp(1365) = 1228.69  
std error est = 0.2      max error est = 1.0

NITROGEN (Monatomic) N 50-1500K

$C_p(T) = 1485.0$  - constant

NITROUS OXIDE - Ideal gas  $N_2O$  200-1365K

$$C_p(T) = 419.153 + 2.2147124T - 2.922847E-03T^2 + 2.51402093E-06T^3$$

$$- 1.21894601E-09T^4 + 2.4536593E-13T^5$$

Cp(200) = 763.42      Cp(800) = 1188.6      Cp(1365) = 1321.25  
std error est = 0.2      max error est = 1.5



NITROUS OXIDE (continued) 200-1365K

$$T(Cp) = 14575.3 - 61.673304Cp + 9.760584E-02Cp^2 - 6.8073563E-05Cp^3 + 1.8008804E-08Cp^4$$

$$T(763.42) = 207 \quad Cp(1188.6) = 798 \quad Cp(1321.25) = 1349$$

$$\text{std error est} = 4.5 \quad \text{max error est} = 15.5$$

n-NONANE - Ideal gas  $C_9H_{20}$  275-755K

$$Cp(T) = 234.445 + 5.1354876T - 6.79961E-04T^2 - 1.0363492E-06T^3$$

$$Cp(275) = 1573.73 \quad Cp(500) = 2502.65 \quad Cp(755) = 3278.13$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 10$$

755-1365K

$$Cp(T) = 4090.2728 - 12.293253T + 3.122246E-02T^2 - 3.12285246E-05T^3 + 1.46875287E-08T^4 - 2.6962143E-12T^5$$

$$Cp(755) = 3277.62 \quad Cp(1000) = 3782.27 \quad Cp(1365) = 4273.54$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

275-755K

$$T(Cp) = -224.99 + 0.4584096Cp - 1.27932559E-04Cp^2 + 2.413833E-08Cp^3$$

$$T(1573.73) = 274 \quad T(2502.65) = 499 \quad T(3278.13) = 753$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 4.5$$

755-1365K

$$T(Cp) = -5895.99 + 5.3023838Cp - 1.510136E-03Cp^2 + 1.5605569E-07Cp^3$$

$$T(3277.62) = 755 \quad T(3782.27) = 999 \quad T(4273.54) = 1364$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 2.5$$

n-OCTANE - Ideal gas  $C_8H_{18}$  275-755K

$$Cp(T) = 214.4198 + 5.356905T - 1.17497E-03T^2 - 6.991155E-07T^3$$

$$Cp(275) = 1584.17 \quad Cp(500) = 2511.74 \quad Cp(755) = 3288.24$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 2.5$$

755-1365K

$$Cp(T) = 2435.9686 - 4.4681947T + 1.6684329E-02T^2 - 1.7885605E-05T^3 + 8.6428202E-09T^4 - 1.614265E-12T^5$$

$$Cp(755) = 3287.84 \quad Cp(1000) = 3795.05 \quad Cp(1365) = 4289.93$$

$$\text{std error est} = 0.3 \quad \text{max error est} = 2.5$$

275-755K

$$T(Cp) = -200.8856 + 0.42218566Cp - 1.119355E-04Cp^2 + 2.1840378E-08Cp^3$$

$$T(1584.17) = 274 \quad T(2511.74) = 499 \quad T(3288.24) = 754$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 3.5$$

755-1365K

$$T(Cp) = -5575.87 + 5.022854Cp - 1.42858E-03Cp^2 + 1.47978204E-07Cp^3$$

$$T(3287.84) = 755 \quad T(3795.05) = 999 \quad T(4289.93) = 1364$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 2.5$$

OXYGEN - Ideal gas  $O_2$  255-590K

$$Cp(T) = 929.247 - 0.3220603T + 1.166523E-03T^2 - 7.1157865E-07T^3$$

$$Cp(255) = 911.18 \quad Cp(375) = 934.99 \quad Cp(590) = 999.15$$

OXYGEN - Ideal gas (continued)

std error est = 0.1

max error est = 1.5

590-1365K

$$C_p(T) = 597.7293 + 1.183704T - 1.156226E-03T^2 + 5.82171E-07T^3 - 1.1772692E-10T^4$$

$$C_p(590) = 998.93$$

$$C_p(1000) = 1089.65$$

$$C_p(1365) = 1131.11$$

std error est = 0.2

max error est = 1.5

255-590K

$$T(C_p) = -236734.7 + 726.57886C_p - 0.744909C_p^2 + 2.5566076E-04C_p^3$$

$$T(911.18) = 258$$

$$T(934.99) = 376$$

$$T(999.15) = 593$$

std error est = 0.9

max error est = 3.0

590-1365K

$$T(C_p) = -140010.9 + 416.5007C_p - 0.4145086C_p^2 + 1.386105E-04C_p^3$$

$$T(998.93) = 588$$

$$T(1089.65) = 999$$

$$T(1131.11) = 1361$$

std error est = 1.3

max error est = 5.5

OXYGEN - Real gas

255-590K

$$C_p(T) = 953.3639 - 0.4638376T + 1.4358763E-03T^2 - 8.748782E-07T^3$$

$$C_p(255) = 913.95$$

$$C_p(450) = 955.68$$

$$C_p(590) = 999.85$$

std error est = 0.2

max error est = 1.5

590-1365K

$$C_p(T) = 219.422 + 3.319747T - 5.8573E-03T^2 + 5.63507E-06T^3$$

$$- 2.77339408E-09T^4 + 5.4687139E-13T^5$$

$$C_p(590) = 999.51$$

$$C_p(1000) = 1090.42$$

$$C_p(1365) = 1132.44$$

std error est = 0.3

max error est = 2.5

255-590K

$$T(C_p) = -295718.67 + 907.2036C_p - 0.92916735C_p^2 + 3.182752E-04C_p^3$$

$$T(913.95) = 262$$

$$T(955.68) = 452$$

$$T(999.85) = 592$$

std error est = 2.7

max error est = 6.5

590-1365K

$$T(C_p) = -132405.2 + 394.1196C_p - 0.392574C_p^2 + 1.3144876E-04C_p^3$$

$$T(999.51) = 588$$

$$T(1090.42) = 1001$$

$$T(1132.44) = 1365$$

std error est = 2.0

max error est = 4.5

OXYGEN (Monatomic) 0

100-1500K

$$C_p(T) = 1585.2189 - 1.215663T + 2.1959047E-03T^2 - 1.99642E-06T^3 + 8.9693573E-10T^4 - 1.5832808E-13T^5$$

$$C_p(100) = 1483.70$$

$$C_p(800) = 1311.40$$

$$C_p(1500) = 1303.03$$

std error est = 2.2

max error est = 4.5

OXYGEN FLUORIDE OF<sub>2</sub>

250-1500K

$$C_p(T) = 332.589 + 2.433234T - 3.634798E-03T^2 + 2.898411E-06T^3 - 1.1968015E-09T^4 + 2.0153116E-13T^5$$

$$C_p(250) = 754.53$$

$$C_p(800) = 1012.72$$

$$C_p(1500) = 1057.85$$

std error est = 0.6

max error est = 2.5

# OXYGEN FLUORIDE (continued)

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K,  $C_p(T) = 473.5175767 + 1.433681085T - 1.2241397E-03T^2 + 3.5368257E-07T^3$ .

n-PENTANE - Ideal gas  $C_5H_{12}$  275-755K

$$C_p(T) = 272.2797 + 4.8751313T - 7.26261E-05T^2 - 1.3441227E-06T^3$$

Cp(255) = 1488.43      Cp(500) = 2523.67      Cp(755) = 3333.14  
std error est = 0.2      max error est = 1.5

755-1365K

$$C_p(T) = 3335.717 - 8.6427T + 2.4429916E-02T^2 - 2.47927E-05T^3 + 1.1664427E-08T^4 - 2.13511208E-12T^5$$

Cp(755) = 3332.45      Cp(1000) = 3859.55      Cp(1365) = 4378.1  
std error est = 0.4      max error est = 1.5

255-755K

$$T(C_p) = -212.8507 + 0.43514236C_p - 1.13646E-04C_p^2 + 2.102165E-08C_p^3$$

T(1488.43) = 252      T(2523.67) = 499      T(3333.14) = 754  
std error est = 0.6      max error est = 2.5

755-1365K

$$T(C_p) = -5111.7 + 4.53933127C_p - 1.2637957E-03C_p^2 + 1.29008845E-07C_p^3$$

T(3332.45) = 755      T(3859.55) = 999      T(4378.1) = 1364  
std error est = 0.6      max error est = 2.5

n-PENTANE - Real gas 275-610K

$$C_p(T) = 568.52265 + 3.2610887T + 2.9780582E-03T^2 - 3.3016552E-06T^3$$

Cp(275) = 1621.87      Cp(475) = 2435.62      Cp(610) = 2916.51  
std error est = 1.1      max error est = 2.5

275-610K

$$T(C_p) = -24.41966 + 0.14680646C_p + 2.40140066E-05C_p^2$$

T(1621.87) = 277      T(2435.62) = 476      T(2916.51) = 608  
std error est = 1.0      max error est = 2.5

1-PENTANOL  $CH_3(CH_2)_4OH$  420-575K

$$\ln[C_p(T)] = 10.279185082 - 1.70935586E-02T + 3.51784187E-05T^2 - 2.23529412E-08T^3$$

Cp(420) = 2098.13      Cp(500) = 2280.35      Cp(575) = 2516.24  
\*\*Note:  $C_p(T) = \exp[fctn(T)]$       max error est = 31.5

3-PENTANONE  $(C_2H_5)_2CO$  275-1275K

$$C_p(T) = 454.357 + 3.5460727T - 7.37756E-06T^2 - 1.42200623E-06T^3 + 5.2151059E-10T^4$$

Cp(275) = 1402.39      Cp(875) = 2904.59      Cp(1275) = 3394.43  
std error est = 7.3      max error est = 15.5

3-PENTANONE (continued) 275-1275K  
 $T(\text{Cp}) = 613.076 - 1.234964\text{Cp} + 1.14343587\text{E-03Cp}^2 - 3.77839\text{E-07Cp}^3$   
 $+ 4.8618495\text{E-11Cp}^4$   
 $T(1402.39) = 276 \quad T(2904.59) = 874 \quad T(3394.43) = 1273$   
 - std error est = 4.6 - - - - - max error est = 12.5

1-PENTENE  $\text{CH}_2\text{CH}(\text{CH}_2)_2\text{CH}_3$  300-1000K  
 $\text{Cp}(T) = -2907.644 + 35.149484T - 0.12403026T^2 + 2.59522805\text{E-04}T^3$   
 $- 3.0126233\text{E-07}T^4 + 1.8150582\text{E-10}T^5 - 4.4468884\text{E-14}T^6$   
 $\text{Cp}(300) = 1450.01 \quad \text{Cp}(600) = 2583.63 \quad \text{Cp}(1000) = 3508.99$   
 std error est = 0.7 max error est = 2.0  
300-1000K  
 $T(\text{Cp}) = 687.768 - 1.0899882\text{Cp} + 8.813122\text{E-04Cp}^2 - 2.5959466\text{E-07Cp}^3$   
 $+ 2.9687246\text{E-11Cp}^4$   
 $T(1450.01) = 300 \quad T(2583.63) = 600 \quad T(3508.99) = 999$   
 - std error est = 1.1 - - - - - max error est = 2.5

1-PENTYNE  $\text{HCCCH}_2\text{CH}_2\text{CH}_3$  300-1500K  
 $\text{Cp}(T) = 728.51 + 0.945078T + 1.1769974\text{E-02}T^2 - 2.4194313\text{E-05}T^3$   
 $+ 2.2017637\text{E-08}T^4 - 9.7690847\text{E-12}T^5 + 1.7071486\text{E-15}T^6$   
 $\text{Cp}(300) = 1573.93 \quad \text{Cp}(600) = 2480.27 \quad \text{Cp}(1500) = 3698.55$   
 std error est = 2.3 max error est = 5.5  
300-1500K  
 $T(\text{Cp}) = 1238.15 - 2.163448\text{Cp} + 1.6002117\text{E-03Cp}^2 - 4.685943\text{E-07Cp}^3$   
 $+ 5.38393765\text{E-11Cp}^4$   
 $T(1573.93) = 301 \quad T(2480.27) = 604 \quad T(3698.55) = 1493$   
 - std error est = 4.9 - - - - - max error est = 10.5

2-PENTYNE  $\text{CH}_3\text{CCCH}_2\text{CH}_3$  300-1500K  
 $\text{Cp}(T) = 452.2996 + 2.3209779T + 5.95716\text{E-03}T^2 - 1.31102\text{E-05}T^3$   
 $+ 1.156122\text{E-08}T^4 - 4.958557\text{E-12}T^5 + 8.4360724\text{E-16}T^6$   
 $\text{Cp}(300) = 1412.97 \quad \text{Cp}(800) = 2741.04 \quad \text{Cp}(1500) = 3574.30$   
 std error est = 2.2 max error est = 4.5  
300-1500K  
 $T(\text{Cp}) = 921.43 - 1.691162\text{Cp} + 1.3965377\text{E-03Cp}^2 - 4.3702767\text{E-07Cp}^3$   
 $+ 5.350453\text{E-11Cp}^4$   
 $T(1412.97) = 300 \quad T(2741.04) = 799 \quad T(3574.30) = 1498$   
 - std error est = 3.9 - - - - - max error est = 7.5

PHOSGENE  $\text{COCl}_2$  100-1500K  
 $\text{Cp}(T) = 191.11 + 2.065565T - 3.2659378\text{E-03}T^2 + 2.8264054\text{E-06}T^3$   
 $- 1.2613311\text{E-09}T^4 + 2.2603022\text{E-13}T^5$

PHOSGENE (continued)

Cp(100) = 367.71      Cp(800) = 757.91      Cp(1500) = 811.14  
 - std error est = 1.8 - - - - - max error est = 3.5 -

PHOSPHINE       $\text{PH}_3$       100-1500K

Cp(T) = 1105.46 - 2.30246882T + 1.2040496E-02T<sup>2</sup> - 1.9018E-05T<sup>3</sup>  
          + 1.541445E-08T<sup>4</sup> - 6.4490826E-12T<sup>5</sup> + 1.0993473E-15T<sup>6</sup>  
 Cp(100) = 978.08      Cp(800) = 1720.90      Cp(1500) = 2142.31  
 - std error est = 1.3 - - - - - max error est = 2.5 -

PHOSPHINE, TRIDEUTERATED       $\text{PD}_3$       300-1000K

Cp(T) = 577.57 + 1.8502044T + 7.1804343E-04T<sup>2</sup> - 2.132996E-06T<sup>3</sup>  
          + 9.1328895E-10T<sup>4</sup>  
 Cp(300) = 1147.06      Cp(700) = 1712.22      Cp(1000) = 1926.11  
 std error est = 0.4      max error est = 1.5  
300-1000K  
 T(Cp) = 4259.23 - 12.773886Cp + 1.4525346E-02Cp<sup>2</sup> - 7.085359E-06Cp<sup>3</sup>  
          + 1.3141044E-09Cp<sup>4</sup>  
 T(1147.06) = 300      T(1712.22) = 700      T(1926.11) = 1000  
 - std error est = 0.9 - - - - - max error est = 3.5 -

PHOSPHORUS TRICHLORIDE       $\text{PCl}_3$       100-1500K

Cp(T) = 118.82 + 2.8526816T - 7.620737E-03T<sup>2</sup> + 1.10669999E-05T<sup>3</sup>  
          - 8.9651026E-09T<sup>4</sup> + 3.799535E-12T<sup>5</sup> - 6.55658E-16T<sup>6</sup>  
 Cp(100) = 338.09      Cp(800) = 591.05      Cp(1500) = 600.84  
 - std error est = 0.6 - - - - - max error est = 1.5 -

PHOSPHORUS TRIFLUORIDE       $\text{PF}_3$       100-1500K

Cp(T) = 250.76 + 1.7158179T - 4.21548E-04T<sup>2</sup> - 3.5547345E-06T<sup>3</sup>  
          + 5.2965343E-09T<sup>4</sup> - 3.00115347E-12T<sup>5</sup> + 6.166475E-16T<sup>6</sup>  
 Cp(100) = 415.07      Cp(800) = 881.29      Cp(1500) = 926.47  
 - std error est = 1.8 - - - - - max error est = 4.5 -

PROPADIENE       $\text{C}(\text{CH}_2)_2$       275-1500K

Cp(T) = 252.095 + 4.5469778T - 4.231012E-04T<sup>2</sup> - 5.3604454E-06T<sup>3</sup>  
          + 6.62186899E-09T<sup>4</sup> - 3.3478109E-12T<sup>5</sup> + 6.3370948E-16T<sup>6</sup>  
 Cp(275) = 1391.92      Cp(800) = 2655.77      Cp(1500) = 3348.20  
 std error est = 0.9      max error est = 3.5  
275-1500K  
 T(Cp) = 1271.52 - 2.4411838Cp + 1.9691654E-03Cp<sup>2</sup> - 6.3636372E-07Cp<sup>3</sup>  
          + 8.1224744E-11Cp<sup>4</sup>  
 T(1391.92) = 278      T(2655.77) = 798      T(3348.20) = 1495

PROPADIENE (continued)

std error est = 3.3 max error est = 7.5

PROPANE - Ideal gas  $C_3H_8$  275-755K

$$Cp(T) = 84.1607 + 5.7701407T - 1.292127E-03T^2 - 6.9945925E-07T^3$$

$$Cp(275) = 1558.69 \quad Cp(500) = 2558.77 \quad Cp(755) = 3403.05$$

$$std\ error\ est = 0.2 \quad max\ error\ est = 1.5$$

755-1365K

$$Cp(T) = 3474.56 - 9.4956207T + 2.643558E-02T^2 - 2.6640384E-05T^3$$

$$+ 1.2466175E-08T^4 - 2.271073E-12T^5$$

$$Cp(755) = 3402.59 \quad Cp(1000) = 3969.24 \quad Cp(1365) = 4529.56$$

$$std\ error\ est = 0.4 \quad max\ error\ est = 1.5$$

275-755K

$$T(Cp) = -134.47 + 0.349Cp - 8.1104732E-05Cp^2 + 1.623344E-08Cp^3$$

$$T(1558.69) = 274 \quad T(2558.77) = 499 \quad T(3403.05) = 754$$

$$std\ error\ est = 0.6 \quad max\ error\ est = 2.5$$

755-1365K

$$T(Cp) = -4331.0 + 3.78505Cp - 1.0204888E-03Cp^2 + 1.02092847E-07Cp^3$$

$$T(3402.59) = 755 \quad T(3969.24) = 999 \quad T(4529.56) = 1364$$

std error est = 0.6 max error est = 2.5

CYCLOPROPANE  $C_3H_8$  100-1000K

$$Cp(T) = 1304.37 - 9.76052T + 5.6216148E-02T^2 - 9.9085315E-05T^3$$

$$+ 7.8256763E-08T^4 - 2.34147557E-11T^5$$

$$Cp(100) = 798.99 \quad Cp(600) = 2604.79 \quad Cp(1000) = 3516.69$$

std error est = 3.3 max error est = 8.5

1,2-PROPANEDIOL  $CH_3CHOHCH_2OH$  275-775K

$$Cp(T) = 840.077 + 1.432479T + 7.47762E-03T^2 - 1.398118E-05T^3$$

$$+ 7.503585E-09T^4$$

$$Cp(275) = 1551.65 \quad Cp(525) = 2200.05 \quad Cp(775) = 2640.29$$

$$std\ error\ est = 3.4 \quad max\ error\ est = 7.5$$

275-775K

$$T(Cp) = -170.21 + 0.384686Cp - 1.377934E-04Cp^2 + 4.859613E-08Cp^3$$

$$T(1551.65) = 276 \quad T(2200.05) = 527 \quad T(2640.29) = 779$$

std error est = 2.1 max error est = 6.5

1-PROPANOL  $CH_3(CH_2)_2OH$  275-1500K

$$Cp(T) = -18.073 + 4.897967T + 4.1591909E-03T^2 - 1.714072E-05T^3$$

$$+ 1.9134617E-08T^4 - 9.587348E-12T^5 + 1.8328355E-15T^6$$

$$Cp(275) = 1382.08 \quad Cp(800) = 2962.56 \quad Cp(1500) = 3779.34$$

$$std\ error\ est = 2.2 \quad max\ error\ est = 4.5$$

275-1500K

$$T(Cp) = 805.72 - 1.316275Cp + 1.03367336E-03Cp^2 - 3.1066055E-07Cp^3$$

$$+ 3.7595022E-11Cp^4$$

1-PROPANOL (continued)

T(1382.08) = 278      T(2962.56) = 797      T(3779.34) = 1495  
std error est = 4.0      max error est = 9.5

2-PROPANOL (CH<sub>3</sub>)<sub>2</sub>CHOH      275-1500K

Cp(T) = 281.08 + 3.55930603T + 5.60782535E-03T<sup>2</sup> - 1.592439E-05T<sup>3</sup>  
+ 1.567946E-08T<sup>4</sup> - 7.2127354E-12T<sup>5</sup> + 1.289756E-15T<sup>6</sup>  
Cp(275) = 1431.69      Cp(800) = 2961.18      Cp(1500) = 3789.51  
std error est = 2.5      max error est = 6.5

275-1500K  
T(Cp) = 712.46 - 1.195778Cp + 9.704307E-04Cp<sup>2</sup> - 2.9394792E-07Cp<sup>3</sup>  
+ 3.576185E-11Cp<sup>4</sup>  
T(1431.69) = 277      T(2961.18) = 798      T(3789.51) = 1495  
std error est = 3.3      max error est = 6.5

PROPYLBENZENE C<sub>6</sub>H<sub>5</sub>(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>      300-1500K

Cp(T) = 156.805 + 2.42815T + 9.353183E-03T<sup>2</sup> - 2.149015E-05T<sup>3</sup>  
+ 1.9780312E-08T<sup>4</sup> - 8.6963805E-12T<sup>5</sup> + 1.499592E-15T<sup>6</sup>  
Cp(300) = 1286.98      Cp(800) = 2727.9      Cp(1500) = 3495.42  
std error est = 1.8      max error est = 4.0

300-1500K  
T(Cp) = 788.38 - 1.415034Cp + 1.254462E-03Cp<sup>2</sup> - 4.2097165E-07Cp<sup>3</sup>  
+ 5.5624451E-11Cp<sup>4</sup>  
T(1286.98) = 300      T(2727.9) = 798      T(3495.42) = 1494  
std error est = 3.9      max error est = 7.5

PROPYL ETHER [CH<sub>3</sub>(CH<sub>2</sub>)<sub>2</sub>]<sub>2</sub>O      275-1275K

Cp(T) = 2220.965 - 15.85878T + 8.362134E-02T<sup>2</sup> - 1.752393E-04T<sup>3</sup>  
+ 1.89973E-07T<sup>4</sup> - 1.0442973E-10T<sup>5</sup> + 2.2914465E-14T<sup>6</sup>  
Cp(275) = 1471.38      Cp(775) = 2885.54      Cp(1275) = 3333.43  
std error est = 9.0      max error est = 21.5

PROPYLENE CH<sub>3</sub>CCH      275-1500K

Cp(T) = 296.204 + 5.18992T - 4.4112215E-03T<sup>2</sup> + 2.621706E-06T<sup>3</sup>  
- 9.5357975E-10T<sup>4</sup> + 1.5122198E-13T<sup>5</sup>  
Cp(275) = 1439.14      Cp(800) = 2626.24      Cp(1500) = 3324.94  
std error est = 0.7      max error est = 3.5

275-1500K  
T(Cp) = 1475.3 - 2.85557Cp + 2.245565E-03Cp<sup>2</sup> - 7.110777E-07Cp<sup>3</sup>  
+ 8.859352E-11Cp<sup>4</sup>  
T(1439.14) = 277      T(2626.24) = 798      T(3324.94) = 1496  
std error est = 2.7      max error est = 7.5

SILANE  $\text{SiH}_4$  100-1500K  
 $\text{Cp}(T) = 1250.39 - 4.4063697T + 0.02678T^2 - 4.8775018E-05T^3$   
 $+ 4.4327926E-08T^4 - 2.0245577E-11T^5 + 3.687426E-15T^6$   
 $\text{Cp}(100) = 1033.1$   $\text{Cp}(800) = 2390.97$   $\text{Cp}(1500) = 2952.51$   
 $\text{std error est} = 5.8$   $\text{max error est} = 20.5$

SILICON TETRACHLORIDE  $\text{SiCl}_4$  100-1500K  
 $\text{Cp}(T) = 112.78 + 2.865988T - 7.278228E-03T^2 + 1.0156921E-05T^3$   
 $- 7.960333E-09T^4 + 3.27887075E-12T^5 - 5.517042E-16T^6$   
 $\text{Cp}(100) = 335.99$   $\text{Cp}(800) = 617.09$   $\text{Cp}(1500) = 630.84$   
 $\text{std error est} = 1.0$   $\text{max error est} = 2.5$

SILICON TETRAFLUORIDE  $\text{SiF}_4$  100-1500K  
 $\text{Cp}(T) = 142.66 + 3.045967T - 5.205945E-03T^2 + 5.425593E-06T^3$   
 $- 3.534804E-09T^4 + 1.32511825E-12T^5 - 2.1643323E-16T^6$   
 $\text{Cp}(100) = 400.28$   $\text{Cp}(800) = 955.15$   $\text{Cp}(1500) = 1011.97$   
 $\text{std error est} = 0.7$   $\text{max error est} = 1.5$

STYRENE  $\text{C}_6\text{H}_5\text{CHCH}_2$  275-1500K  
 $\text{Cp}(T) = -126.7 + 4.27917184T + 2.927387E-03T^2 - 1.2277425E-05T^3$   
 $+ 1.2935809E-08T^4 - 6.1243779E-12T^5 + 1.11436976E-15T^6$   
 $\text{Cp}(275) = 1080.96$   $\text{Cp}(800) = 2467.92$   $\text{Cp}(1500) = 3116.28$   
 $\text{std error est} = 1.1$   $\text{max error est} = 2.5$

275-1500K  
 $T(\text{Cp}) = 913.36 - 1.888481\text{Cp} + 1.8311187E-03\text{Cp}^2 - 6.899175E-07\text{Cp}^3$   
 $+ 1.01386298E-10\text{Cp}^4$   
 $T(1080.96) = 279$   $T(2467.92) = 796$   $T(3116.28) = 1493$   
 $\text{std error est} = 4.5$   $\text{max error est} = 10.5$

SULFUR  $\text{S}_2$  275-1500K  
 $\text{Cp}(T) = 376.86 + 0.6300876T - 7.88127E-04T^2 + 4.5750016E-07T^3$   
 $- 1.0076704E-10T^4$   
 $\text{Cp}(275) = 499.46$   $\text{Cp}(800) = 569.24$   $\text{Cp}(1500) = 580.95$   
 $\text{std error est} = 0.5$   $\text{max error est} = 2.5$

Note: For  $T(\text{Cp})$  calculations, use the iterative procedures discussed in Section 5 and the following eqn: 275-1500K,  $\text{Cp}(T) =$   
 $409.44875 + 0.421901486T - 3.57102338E-04T^2 + 1.02449694E-07T^3$

SULFUR (Monatomic) S 100-1500K  
 $\text{Cp}(T) = 504.485 + 2.3393178T - 8.5202771E-03T^2 + 1.43794546E-05T^3$   
 $- 1.26931826E-08T^4 + 5.67465485E-12T^5 - 1.0136105E-15T^6$   
 $\text{Cp}(100) = 666.38$   $\text{Cp}(800) = 679.87$   $\text{Cp}(1500) = 660.51$   
 $\text{std error est} = 1.2$   $\text{max error est} = 3.0$



SULFUR DICHLORIDE  $\text{SCl}_2$  100-1500K

$$\begin{aligned} \text{Cp}(T) &= 239.65 + 1.59183756T - 3.52713\text{E-}03T^2 + 4.2688109\text{E-}06T^3 \\ &\quad - 2.9106702\text{E-}09T^4 + 1.0505776\text{E-}12T^5 - 1.5627007\text{E-}16T^6 \\ \text{Cp}(100) &= 367.55 \quad \text{Cp}(800) = 552.47 \quad \text{Cp}(1500) = 561.14 \\ \text{std error est} &= 0.9 \quad \text{max error est} = 2.5 \end{aligned}$$

SULFUR DIFLUORIDE  $\text{SF}_2$  100-1500K

$$\begin{aligned} \text{Cp}(T) &= 446.1812 - 0.070297366T + 4.760524\text{E-}03T^2 - 1.189425\text{E-}05T^3 \\ &\quad + 1.2720916\text{E-}08T^4 - 6.4083936\text{E-}12T^5 + 1.2442913\text{E-}15T^6 \\ \text{Cp}(100) &= 476.07 \quad \text{Cp}(800) = 783.59 \quad \text{Cp}(1500) = 817.97 \\ \text{std error est} &= 3.5 \quad \text{max error est} = 8.0 \end{aligned}$$

SULFUR DIOXIDE  $\text{SO}_2$  300-1365K

Ideal gas

$$\begin{aligned} \text{Cp}(T) &= 432.805 + 0.5994156T + 4.593367\text{E-}04T^2 - 1.433024\text{E-}06T^3 \\ &\quad + 1.0409341\text{E-}09T^4 - 2.5313735\text{E-}13T^5 \\ \text{Cp}(300) &= 623.09 \quad \text{Cp}(700) = 793.33 \quad \text{Cp}(1365) = 876.40 \\ \text{std error est} &= 0.3 \quad \text{max error est} = 1.5 \end{aligned}$$

300-1365K

$$\begin{aligned} T(\text{Cp}) &= 155222.71 - 877.595265\text{Cp} + 1.857197245\text{Cp}^2 - 1.7428909\text{E-}03\text{Cp}^3 \\ &\quad + 6.1359879\text{E-}07\text{Cp}^4 \end{aligned}$$

$$\begin{aligned} T(623.09) &= 309 \quad T(793.33) = 696 \quad T(876.40) = 1342 \\ \text{std error est} &= 5.5 \quad \text{max error est} = 23.5 \end{aligned}$$

SULFUR HEXAFLUORIDE  $\text{SF}_6$  100-1500K

$$\begin{aligned} \text{Cp}(T) &= 24.233 + 2.33532T + 1.4344428\text{E-}03T^2 - 1.05440664\text{E-}05T^3 \\ &\quad + 1.3847595\text{E-}08T^4 - 7.6376433\text{E-}12T^5 + 1.56118585\text{E-}15T^6 \\ \text{Cp}(100) &= 262.88 \quad \text{Cp}(800) = 990.5 \quad \text{Cp}(1500) = 1056.46 \\ \text{std error est} &= 5.7 \quad \text{max error est} = 11.5 \end{aligned}$$

SULFUR MONOCHLORIDE  $\text{S}_2\text{Cl}_2$  100-1500K

$$\begin{aligned} \text{Cp}(T) &= 150.63 + 2.756806T - 7.3955367\text{E-}03T^2 + 1.07461656\text{E-}05T^3 \\ &\quad - 8.69281614\text{E-}09T^4 + 3.6742817\text{E-}12T^5 - 6.31809797\text{E-}16T^6 \\ \text{Cp}(100) &= 362.27 \quad \text{Cp}(800) = 602.75 \quad \text{Cp}(1500) = 611.68 \\ \text{std error est} &= 0.9 \quad \text{max error est} = 2.5 \end{aligned}$$

SULFUR MONOXIDE  $\text{SO}$  300-1500K

$$\begin{aligned} \text{Cp}(T) &= 498.98 + 0.54531131T - 3.97417036\text{E-}04T^2 + 1.0243734\text{E-}07T^3 \\ \text{Cp}(300) &= 629.57 \quad \text{Cp}(900) = 742.53 \quad \text{Cp}(1500) = 768.48 \\ \text{std error est} &= 0.7 \quad \text{max error est} = 2.0 \end{aligned}$$

300-1500K

$$\begin{aligned} T(\text{Cp}) &= 2673548.1 - 15732.3334\text{Cp} + 34.6862568\text{Cp}^2 - 3.3963896\text{E-}02\text{Cp}^3 \\ &\quad + 1.24657038\text{E-}05\text{Cp}^4 \end{aligned}$$

$$T(629.57) = 301 \quad T(742.53) = 902 \quad T(768.48) = 1513$$

SULFUR MONOXIDE (continued)

std error est = 2.5 max error est = 15.5

SULFUR TETRAFLUORIDE  $\text{SF}_4$  100-1500K

$$\ln[\text{Cp}(T)] = 5.4481069265 + 5.31628197\text{E-}03T - 7.63297357\text{E-}06T^2 \\ + 4.87033913\text{E-}09T^3 - 1.14651855\text{E-}12T^4$$

$$\text{Cp}(200) = 514.49 \quad \text{Cp}(800) = 934.52 \quad \text{Cp}(1500) = 974.07$$

\*\*Note: Cp(T) = exp[fctn(T)] max error est = 15.5

SULFUR TRIOXIDE  $\text{SO}_3$  100-1500K

$$\text{Cp}(T) = 332.45 + 0.76715644T + 2.18883267\text{E-}03T^2 - 6.4464146\text{E-}06T^3 \\ + 6.8053136\text{E-}09T^4 - 3.3274957\text{E-}12T^5 + 6.2860794\text{E-}16T^6$$

$$\text{Cp}(100) = 425.26 \quad \text{Cp}(800) = 908.35 \quad \text{Cp}(1500) = 995.38$$

std error est = 1.4 max error est = 3.5

SULFURYL FLUORIDE  $\text{SO}_2\text{F}_2$  100-1500K

$$\text{Cp}(T) = 188.38 + 1.51815532T + 1.6848848\text{E-}03T^2 - 8.08750268\text{E-}06T^3 \\ + 9.88024136\text{E-}09T^4 - 5.25778454\text{E-}12T^5 + 1.0506054\text{E-}15T^6$$

$$\text{Cp}(100) = 349.89 \quad \text{Cp}(800) = 939.92 \quad \text{Cp}(1500) = 1020.75$$

std error est = 3.2 max error est = 7.5

THIONYL CHLORIDE  $\text{SOCl}_2$  100-1500K

$$\text{Cp}(T) = 126.39 + 3.01522T - 8.0321113\text{E-}03T^2 + 1.2067313\text{E-}05T^3 \\ - 1.01854131\text{E-}08T^4 + 4.48266475\text{E-}12T^5 - 7.98302653\text{E-}16T^6$$

$$\text{Cp}(100) = 358.68 \quad \text{Cp}(800) = 664.14 \quad \text{Cp}(1500) = 687.57$$

std error est = 1.4 max error est = 3.5

THIONYL FLUORIDE  $\text{SOF}_2$  100-1500K

$$\text{Cp}(T) = 252.57 + 1.591359T + 9.12985723\text{E-}05T^2 - 4.47083245\text{E-}06T^3 \\ + 6.1962479\text{E-}09T^4 - 3.45812419\text{E-}12T^5 + 7.09108083\text{E-}16T^6$$

$$\text{Cp}(100) = 408.73 \quad \text{Cp}(800) = 885.74 \quad \text{Cp}(1500) = 941.53$$

std error est = 2.3 max error est = 5.5

THIOPHOSGENE  $\text{CSCl}_2$  275-1000K

$$\text{Cp}(T) = 59.14 + 3.3998836T - 8.5876389\text{E-}03T^2 + 1.1794626\text{E-}05T^3 \\ - 8.30715093\text{E-}09T^4 + 2.33820883\text{E-}12T^5$$

$$\text{Cp}(275) = 546.13 \quad \text{Cp}(600) = 660.37 \quad \text{Cp}(1000) = 697.07$$

std error est = 0.7 max error est = 2.5

275-1000K

$$T(\text{Cp}) = 488250.36 - 3272.97043\text{Cp} + 8.22103684\text{Cp}^2 - 9.17008593\text{E-}03\text{Cp}^3 \\ + 3.83549875\text{E-}06\text{Cp}^4$$

$$T(546.13) = 277 \quad T(660.37) = 589 \quad T(697.07) = 989$$

std error est = 9.4 max error est = 21.5

TOLUENE  $C_7H_8$  275-755K  
 Ideal gas  
 $Cp(T) = -310.29 + 5.640685T - 2.81410224E-03T^2 + 2.4913887E-07T^3$   
 $Cp(275) = 1033.26$   $Cp(500) = 1837.67$   $Cp(755) = 2451.54$   
 std error est = 0.2 max error est = 2.0  
755-1365K  
 $Cp(T) = 109.89 + 4.64889983T - 2.404749E-03T^2 + 4.70371704E-07T^3$   
 $Cp(755) = 2451.48$   $Cp(1000) = 2824.41$   $Cp(1365) = 3171.35$   
 std error est = 0.2 max error est = 2.0  
275-755K  
 $T(Cp) = -62.5 + 0.441587267Cp - 1.62355359E-04Cp^2 + 4.8116433E-08Cp^3$   
 $T(1033.26) = 274$   $T(1837.67) = 499$   $T(2451.54) = 753$   
 std error est = 0.7 max error est = 3.0  
755-1365K  
 $T(Cp) = -6732.5 + 8.1967182Cp - 3.1808569E-03Cp^2 + 4.4184319E-07Cp^3$   
 $T(2451.48) = 755$   $T(2824.41) = 999$   $T(3171.35) = 1364$   
 std error est = 0.9 max error est = 2.5

TOLUENE - Real gas 300-610K  
 $Cp(T) = 8.203797 + 4.000876T + 1.11409614E-04T^2 - 1.5192015E-06T^3$   
 $Cp(300) = 1177.48$   $Cp(450) = 1692.72$   $Cp(610) = 2145.36$   
 std error est = 1.2 max error est = 3.0  
300-610K  
 $T(Cp) = -91.3 + 0.44221698Cp - 1.4179088E-04Cp^2 + 4.0999999E-08Cp^3$   
 $T(1177.48) = 300$   $T(1692.72) = 450$   $T(2145.36) = 610$   
 std error est = 0.6 max error est = 2.5

1,1,1-TRICHLOROETHANE  $CH_3CCl_3$  300-600K  
 $Cp(T) = 558.306\exp(0.0011T)$   
 $Cp(300) = 776.59$   $Cp(450) = 915.9$   $Cp(600) = 1080.21$   
 \*\*Note: The accuracy of this fit is within 5.0% of the reference  
 source values. The estimated maximum error is 45.

TRICHLOROFLUORO-  $CCl_3F$  90-700K (FREON-11)  
 METHANE - Ideal gas  
 $Cp(T) = 88.42 + 2.6878447T - 4.66910945E-03T^2 + 3.96538806E-06T^3$   
 $- 1.311654E-09T^4$   
 $Cp(90) = 295.31$   $Cp(450) = 660.02$   $Cp(700) = 727.25$   
 std error est = 0.3 max error est = 2.5  
700-1365K  
 $Cp(T) = 398.846 + 0.85444834T - 6.7934387E-04T^2 + 1.8385308E-07T^3$   
 $Cp(700) = 727.14$   $Cp(1000) = 757.8$   $Cp(1365) = 766.99$   
 std error est = 0.2 max error est = 2.5

TRICHLOROFLUOROMETHANE (FREON-11) (continued)

$$T(Cp) = 1858.9 - 17.09586Cp + \frac{90-700K}{5.92007E-02Cp^2} - 8.71182475E-05Cp^3 + 4.813565E-08Cp^4$$

T(295.31) = 96      T(660.02) = 451      T(727.25) = 693  
std error est = 3.8      max error est = 9.5

Note: For T(Cp) calculations from 700-1365K, use the iterative procedures discussed in Section 5 and the following equations:  
700-1365K,  $Cp(T) = 573.5800054 + 0.306189477T - 1.21913823E-04T^2$ .

TRICHLOROTRIFLUORO-  $C_2Cl_3F_3$  320-465K

ETHANE (FREON-113)

$$Cp(T) = 953.33 - 4.1752099T + 1.48443126E-02T^2 - 1.4511695E-05T^3$$

Cp(320) = 661.80      Cp(425) = 746.12      Cp(465) = 762.5  
std error est = 0.1      max error est = 1.5

$$T(Cp) = -39428.5 + 169.22394Cp - \frac{320-465K}{0.2413860737Cp^2} + 1.1549402E-04Cp^3$$

T(661.80) = 318      T(746.12) = 426      T(762.5) = 462  
std error est = 1.7      max error est = 4.5

TRICHLOROSILANE  $SiHCl_3$  100-1000K

$$Cp(T) = 163.34 + 2.096026T - 3.3286844E-03T^2 + 2.57996254E-06T^3 - 7.76498622E-10T^4$$

Cp(100) = 342.16      Cp(600) = 679.27      Cp(1000) = 734.15  
std error est = 1.5      max error est = 3.5

$$T(Cp) = 9037.45 - 76.410239Cp + \frac{100-1000K}{0.238723665Cp^2} - 3.24312525E-04Cp^3 + 1.64234225E-07Cp^4$$

T(342.16) = 101      T(679.27) = 602      T(734.15) = 990  
std error est = 8.9      max error est = 15.5

1,1,1-TRICHLORO-2,2,2-TRI-  $CF_3CCl_3$  200-800K  
FLUOROETHANE

$$Cp(T) = 185.89 + 1.4044747T + 2.6500078E-03T^2 - 1.18943003E-05T^3 + 1.45980328E-08T^4 - 6.1337978E-12T^5$$

Cp(200) = 499.02      Cp(500) = 784.54      Cp(800) = 885.02  
std error est = 0.7      max error est = 2.0

$$T(Cp) = 7781.2 - 49.265363Cp + \frac{200-800K}{0.117538654Cp^2} - 1.2291743E-04Cp^3 + 4.8509877E-08Cp^4$$

T(499.02) = 200      T(784.54) = 498      T(885.02) = 798  
std error est = 4.3      max error est = 9.5

1,1,1-TRIFLUOROETHANE  $CH_3CF_3$  100-1500K

1,1,1-TRIFLUOROETHANE (continued)

$$\begin{aligned} \text{Cp}(T) &= 264.398 + 1.8040847T + 4.17525467E-03T^2 - 1.2539045E-05T^3 \\ &\quad + 1.3278592E-08T^4 - 6.49158273E-12T^5 + 1.2220205E-15T^6 \\ \text{Cp}(100) &= 475.28 \quad \text{Cp}(800) = 1591.93 \quad \text{Cp}(1500) = 1892.56 \\ \text{std error est} &= 1.7 \quad \text{max error est} = 3.5 \end{aligned}$$

TRIFLUOROIODOMETHANE  $\text{CF}_3\text{I}$  100-1000K

$$\begin{aligned} \text{Cp}(T) &= 103.14 + 1.255612T - 1.56065E-03T^2 + 9.460232E-07T^3 \\ &\quad - 2.27049635E-10T^4 \\ \text{Cp}(100) &= 214.02 \quad \text{Cp}(600) = 469.59 \quad \text{Cp}(1000) = 517.08 \\ \text{std error est} &= 0.4 \quad \text{max error est} = 2.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1000K,  $\text{Cp}(T) = 110.51576796 + 1.161867871T - 1.20896094E-03T^2 + 4.5474783E-07T^3$ .

TRIMETHYLAMINE  $(\text{CH}_3)_3\text{N}$  275-1475K

$$\begin{aligned} \text{Cp}(T) &= 773.274 - 1.34861408T + 2.365832E-02T^2 - 4.5452006E-05T^3 \\ &\quad + 4.1145841E-08T^4 - 1.84648686E-11T^5 + 3.29518026E-15T^6 \\ \text{Cp}(275) &= 1454.01 \quad \text{Cp}(875) = 3384.35 \quad \text{Cp}(1475) = 4173.36 \\ \text{std error est} &= 2.1 \quad \text{max error est} = 5.5 \end{aligned}$$

275-1475K

$$\begin{aligned} T(\text{Cp}) &= 430.45 - 0.63430825\text{Cp} + 5.6407771E-04\text{Cp}^2 - 1.6640782E-07\text{Cp}^3 \\ &\quad + 1.9643825E-11\text{Cp}^4 \\ T(1454.01) &= 277 \quad T(3384.35) = 871 \quad T(4173.36) = 1471 \\ \text{std error est} &= 3.4 \quad \text{max error est} = 7.5 \end{aligned}$$

2,3,4-TRIMETHYL-  $[(\text{CH}_3)_2\text{CH}]_2\text{CHCH}_3$  400-520K  
PENTANE

$$\begin{aligned} \text{Cp}(T) &= 686.88 + 3.789T \quad T(\text{Cp}) = [\text{Cp} - 686.88]/3.789 \\ \text{There are only three data points in the reference source. The} \\ \text{accuracy of this fit cannot be adequately established.} \end{aligned}$$

WATER - Ideal gas  $\text{H}_2\text{O}$  275-1365K

$$\begin{aligned} \text{Cp}(T) &= 1997.22 - 1.5513626T + 5.4600474E-03T^2 - 7.4448866E-06T^3 \\ &\quad + 5.92340976E-09T^4 - 2.54654038E-12T^5 + 4.50326153E-16T^6 \\ \text{Cp}(275) &= 1858.75 \quad \text{Cp}(800) = 2148.61 \quad \text{Cp}(1365) = 2527.54 \\ \text{std error est} &= 0.6 \quad \text{max error est} = 3.5 \end{aligned}$$

275-1365K

$$\begin{aligned} T(\text{Cp}) &= -138783.1 + 243.21339\text{Cp} - 0.1601304\text{Cp}^2 + 4.6992596E-05\text{Cp}^3 \\ &\quad - 5.155188E-09\text{Cp}^4 \\ T(1858.75) &= 292 \quad T(2148.61) = 798 \quad T(2527.54) = 1360 \\ \text{std error est} &= 5.0 \quad \text{max error est} = 18.5 \end{aligned}$$

WATER - Real gas

375-545K

$$C_p(T) = -9151.27 + 124.55666T - 0.43018315T^2 + 2.5078185E-04T^3 \\ + 1.51700823E-06T^4 - 3.1440734E-09T^5 + 1.82314019E-12T^6$$

Cp(375) = 2041.49      Cp(500) = 1976.29      Cp(545) = 1990.98  
std error est = 0.5      max error est = 2.5

535-1365K

$$C_p(T) = 1855.87 - 0.12328108T + 8.33819257E-04T^2 - 2.7862857E-07T^3$$

Cp(535) = 1985.91      Cp(1000) = 2287.78      Cp(1365) = 2532.55  
std error est = 0.2      max error est = 1.5

Note: For T(Cp) calculations between 375-545K, use the iterative procedures discussed in Section and the following eqn: 375-545K,  
 $C_p(T) = 7288.57944 - 31.60499289T + 6.19666037E-02T^2 - 4.001532E-05T^3$ .

535-1365K

$$T(C_p) = -20093.67 + 24.866517C_p - 1.0260634E-02C_p^2 + 1.495574E-06C_p^3$$

T(1985.91) = 536      T(2287.78) = 1000      T(2532.55) = 1365  
std error est = 0.7      max error est = 3.5

WATER, DIDEUTERATED      D<sub>2</sub>O      0-1500K

$$C_p(T) = 1692.39 + 0.531928T + 9.981787E-04T^2 - 1.32271877E-06T^3 \\ + 6.3221224E-10T^4 - 1.140281E-13T^5$$

Cp(1) = 1692.92      Cp(750) = 2267.77      Cp(1500) = 2606.68  
std error est = 1.5      max error est = 3.5

0-1500K

$$T(C_p) = -262435.28 + 620.045026C_p - 0.58727707C_p^2 + 2.7838713E-04C_p^3 \\ - 6.59628036E-08C_p^4 + 6.2551268E-12C_p^5$$

T(1692.92) = 0      T(2267.77) = 753      T(2606.68) = 1499  
std error est = 1.2      max error est = 5.5

XENON - Ideal gas      Xe      ALL TEMPERATURES

Cp(T) = 158.416 - constant

m-XYLENE      C<sub>6</sub>H<sub>4</sub>(CH<sub>3</sub>)<sub>2</sub>      300-1500K

$$C_p(T) = 112.448 + 2.48622T + 8.20559E-03T^2 - 1.897328E-05T^3 \\ + 1.749458E-08T^4 - 7.7581914E-12T^5 + 1.35754047E-15T^6$$

Cp(300) = 1208.38      Cp(800) = 2618.13      Cp(1500) = 3385.32  
std error est = 1.4      max error est = 3.5

300-1500K

$$T(C_p) = 793.3 - 1.4795435C_p + 1.3653586E-03C_p^2 - 4.736549E-07C_p^3 \\ + 6.4258022E-11C_p^4$$

T(1208.38) = 300      T(2618.13) = 798      T(3385.32) = 1495  
std error est = 3.8      max error est = 8.5

o-XYLENE  $C_6H_4(CH_3)_2$  300-1500K

$$Cp(T) = 220.54 + 2.315837T + 8.00889E-03T^2 - 1.8267628E-05T^3 \\ + 1.67967527E-08T^4 - 7.4499897E-12T^5 + 1.30510608E-15T^6$$

Cp(300) = 1261.77      Cp(800) = 2626.74      Cp(1500) = 3387.23  
std error est = 1.0      max error est = 3.5

300-1500K

$$T(Cp) = 884.7 - 1.6751046Cp + 1.49528125E-03Cp^2 - 5.09322185E-07Cp^3 \\ + 6.778076E-11Cp^4$$

T(1261.77) = 300      T(2626.74) = 798      T(3387.23) = 1495

- std error est = 3.7 - - - - - max error est = 8.5

p-XYLENE  $C_6H_4(CH_3)_2$  300-1500K

$$Cp(T) = 240.04 + 1.4903657T + 1.0968075E-02T^2 - 2.28936254E-05T^3 \\ + 2.05420776E-08T^4 - 8.9907546E-12T^5 + 1.56029453E-15T^6$$

Cp(300) = 1201.83      Cp(800) = 2607.33      Cp(1500) = 3381.23  
std error est = 0.9      max error est = 3.5

300-1500K

$$T(Cp) = -1458.07 + 4.050261Cp - 3.859663E-03Cp^2 + 1.9113335E-06Cp^3 \\ - 4.63203445E-10Cp^4 + 4.53602623E-14Cp^5$$

T(1201.83) = 300      T(2607.33) = 801      T(3381.23) = 1499

- std error est = 1.5 - - - - - max error est = 4.5

APPENDIX B  
TABLE B-I  
SUMMARY OF CONTENTS

THERMAL CONDUCTIVITY FOR  
GASEOUS ELEMENTS AND COMPOUNDS

NAME	FORMULA	APP B PAGE
Acetone	$C_3H_6O$	B-1
Acetylene	$C_2H_2$	B-1
Air	-	B-1
Ammonia	$NH_3$	B-1
Argon	Ar	B-2
Benzene	$C_6H_6$	B-2
Boron Trifluoride	$BF_3$	B-2
Bromine	$Br_2$	B-3
iso-Butane	$i-C_4H_{10}$	B-3
n-Butane	$n-C_4H_{10}$	B-3
Carbon Dioxide	$CO_2$	B-3
Carbon Monoxide	CO	B-4
Carbon Tetrachloride	$CCl_4$	B-4
Chlorine	$Cl_2$	B-4
Chlorodifluoromethane (FREON-22)	$CHClF_2$	B-5
Chloroform	$CHCl_3$	B-5
Chlorotrifluoromethane (FREON-13)	$CClF_3$	B-5
n-Decane	$C_{10}H_{22}$	B-5
Deuterium	$D_2$	B-5
Dichlorodifluoromethane (FREON-12)	$CCl_2F_2$	B-6
Dichlorofluoromethane (FREON-21)	$CHCl_2F$	B-6
Dichlorotetrafluoroethane (FREON-114)	$C_2Cl_2F_4$	B-6
Ethane	$C_2H_6$	B-6
Ethyl Alcohol	$C_2H_5OH$	B-7
Ethyl Ether	$C_4H_{10}O$	B-7
Ethylene	$C_2H_4$	B-7
Fluorine	$F_2$	B-7
Helium	He	B-7
n-Heptane	$C_7H_{16}$	B-8
n-Hexane	$C_6H_{14}$	B-8
Hydrogen	$H_2$	B-8
Hydrogen Chloride	HCl	B-9
Hydrogen Iodide	HI	B-9
Hydrogen Sulfide	$H_2S$	B-10



TABLE B-I  
(CONT.)

NAME	FORMULA	APP B PAGE
Krypton	Kr	B-10
Methane	CH <sub>4</sub>	B-10
Methyl Alcohol	CH <sub>3</sub> OH	B-10
Methyl Chloride	CH <sub>3</sub> Cl	B-10
Neon	Ne	B-11
Nitric Oxide	NO	B-11
Nitrogen	N <sub>2</sub>	B-11
Nitrogen Peroxide	NO <sub>2</sub>	B-12
Nitrous Oxide	N <sub>2</sub> O	B-12
n-Nonane	C <sub>9</sub> H <sub>20</sub>	B-12
n-Octane	C <sub>8</sub> H <sub>18</sub>	B-13
Oxygen	O <sub>2</sub>	B-13
n-Pentane	C <sub>5</sub> H <sub>12</sub>	B-13
Propane	C <sub>3</sub> H <sub>8</sub>	B-13
Radon	Rn	B-14
Sulfur Dioxide	SO <sub>2</sub>	B-14
Toluene	C <sub>7</sub> H <sub>8</sub>	B-14
Trichlorofluoromethane (FREON-11)	CCl <sub>3</sub> F	B-14
Trichlorotrifluoroethane (FREON-113)	C <sub>2</sub> Cl <sub>3</sub> F <sub>3</sub>	B-15
Water (steam)	H <sub>2</sub> O	B-15
Xenon	Xe	B-15

APPENDIX B  
FORMAT EXAMPLE

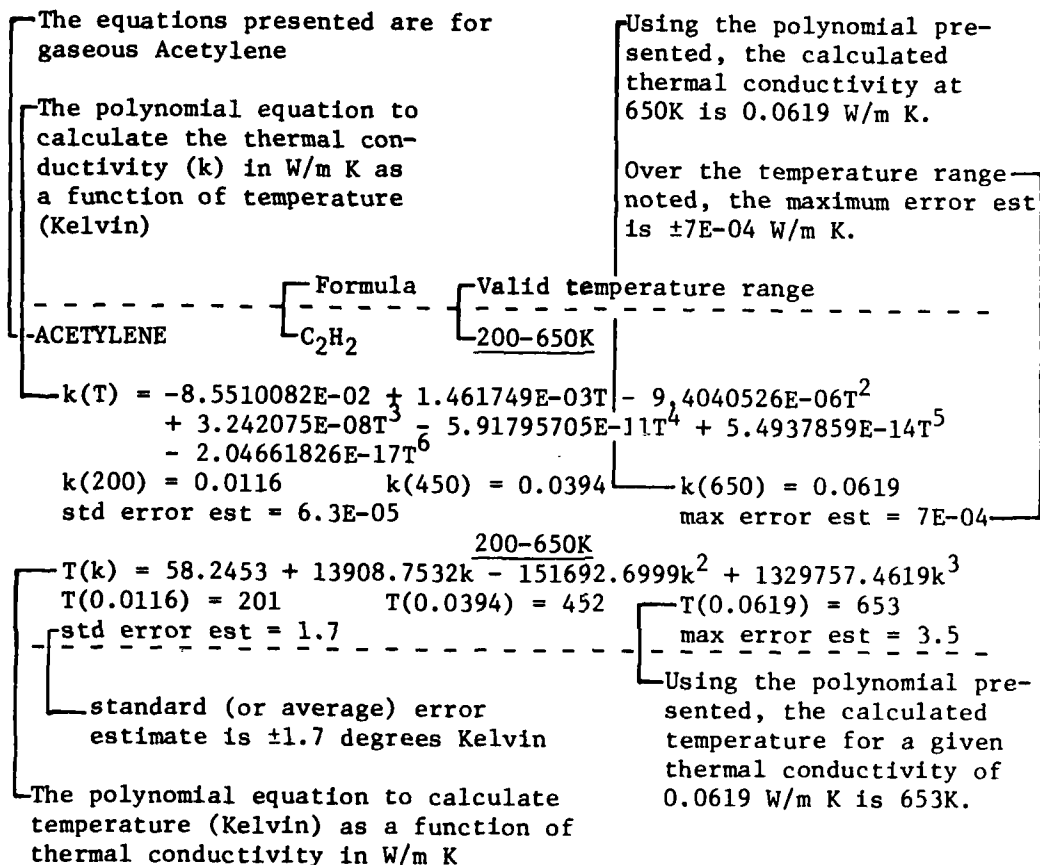


FIGURE B-1

# APPENDIX B

## THERMAL CONDUCTIVITY FOR GASEOUS ELEMENTS AND COMPOUNDS

ACETONE	C <sub>3</sub> H <sub>6</sub> O	280-500K
$k(T) = -4.11573122E-04 + 4.79793901E-06T + 1.15976849E-07T^2$ $k(280) = 0.01002 \quad k(400) = 0.02006 \quad k(500) = 0.03098$ $\text{std error est} = 1.8E-05 \quad \text{max error est} = 4.0E-05$		
$T(k) = 136.464 + 15795.28787k - 132356.15338k^2$ $T(0.01002) = 281 \quad T(0.02006) = 400 \quad T(0.03098) = 499$ $\text{std error est} = 0.7 \quad \text{max error est} = 2.5$		
ACETYLENE	C <sub>2</sub> H <sub>2</sub>	200-650K
$k(T) = -8.5510082E-02 + 1.461749E-03T - 9.4040526E-06T^2$ $+ 3.242075E-08T^3 - 5.91795705E-11T^4 + 5.4937859E-14T^5$ $- 2.04661826E-17T^6$ $k(200) = 0.0116 \quad k(450) = 0.0394 \quad k(650) = 0.0619$ $\text{std error est} = 6.3E-05 \quad \text{max error est} = 7E-04$		
$T(k) = 58.2453 + 13908.7532k - 151692.6999k^2 + 1329757.4619k^3$ $T(0.0116) = 201 \quad T(0.0394) = 452 \quad T(0.0619) = 653$ $\text{std error est} = 1.7 \quad \text{max error est} = 3.5$		
AIR		100-1500K
$k(T) = -2.276501E-03 + 1.2598485E-04T - 1.4815235E-07T^2$ $+ 1.73550646E-10T^3 - 1.066657E-13T^4 + 2.47663035E-17T^5$ $k(100) = 9.0E-02 \quad k(800) = 0.0570 \quad k(1500) = 0.0872$ $\text{std error est} = 1.2E-04 \quad \text{max error est} = 2.5E-04$		
$T(k) = -21.25887 + 12111.0665k - 2060.85234k^2 + 726814.383446k^3$ $T(.009) = 88 \quad T(.0570) = 797 \quad T(.0872) = 1501$ $\text{std error est} = 5.0 \quad \text{max error est} = 13.5$		
AMMONIA	NH <sub>3</sub>	250-900K
$k(T) = 3.25332857E-02 - 2.56604839E-04T + 1.19984154E-06T^2$ $- 1.8411802E-09T^3 + 1.450888E-12T^4 - 4.5463777E-16T^5$ $k(250) = 0.0198 \quad k(650) = 0.0733 \quad k(900) = 0.1147$ $\text{std error est} = 8.8E-05 \quad \text{max error est} = 2E-04$		
$T(k) = 59.78 + 10975.1917k - 54118.9276k^2 + 195945.59072k^3$ $T(.0198) = 257 \quad T(.0733) = 651 \quad T(.1147) = 902$ $\text{std error est} = 2.1 \quad \text{max error est} = 4.5$		

ARGON

Ar

100-2000K

$$k(T) = -5.2839462E-04 + 7.60706705E-05T - 6.4749393E-08T^2 \\ + 5.41874502E-11T^3 - 3.22024235E-14T^4 + 1.17962552E-17T^5 \\ - 1.86231745E-21T^6$$

$$k(100) = 6.48E-03 \quad k(800) = 0.03682 \quad k(2000) = 0.06921 \\ \text{std error est} = 4.6E-05 \quad \text{max error est} = 1E-04$$

2000-6000K

$$k(T) = 1.93082997E-02 + 2.51961654E-05T - 1.67510345E-10T^2 \\ + 1.34423776E-14T^3$$

$$k(2000) = 0.06914 \quad k(4000) = 0.11827 \quad k(6000) = 0.16736 \\ \text{std error est} = 6.2E-05 \quad \text{max error est} = 1E-04$$

6000-10000K

$$k(T) = 9.646322815 - 8.33091359E-03T + 2.95984109E-06T^2 \\ - 5.46353403E-10T^3 + 5.53001474E-14T^4 - 2.90734681E-18T^5 \\ + 6.22212377E-23T^6$$

$$k(6000) = 0.16724 \quad k(8000) = 0.2483 \quad k(10000) = 0.4559 \\ \text{std error est} = 2.9E-04 \quad \text{max error est} = 4E-04$$

100-2000K

$$T(k) = 6.817 + 13959.6435k + 48739.9133k^2 + 6473513.547817k^3 \\ - 59362842.0531k^4$$

$$T(6.48E-03) = 101 \quad T(0.03682) = 801 \quad T(0.06921) = 1990 \\ \text{std error est} = 2.5 \quad \text{max error est} = 11$$

2000-6000K

$$T(k) = -806.5 + 40519.97783k + 982.79608093k^2$$

$$T(0.06914) = 2000 \quad T(0.11827) = 4000 \quad T(0.16736) = 6002$$

$$\text{std error est} = 2.6 \quad \text{max error est} = 5.0$$

BENZENE

C<sub>6</sub>H<sub>6</sub>

250-600K

$$k(T) = 1.26398664E-02 - 8.09524147E-05T + 2.45397874E-07T^2$$

$$k(250) = 7.74E-03 \quad k(450) = 0.0259 \quad k(600) = 0.05241 \\ \text{std error est} = 5E-05 \quad \text{max error est} = 1E-04$$

250-600K

$$T(k) = 119.7 + 20654.901668k - 382444.26277k^2 + 3143235.5389k^3$$

$$T(7.74E-03) = 258 \quad T(0.0259) = 453 \quad T(0.05241) = 604$$

$$\text{std error est} = 2.9 \quad \text{max error est} = 8.5$$

BORON TRIFLUORIDE BF<sub>3</sub>

250-400K

$$k(T) = -0.013508927 + 1.74995767E-04T - 2.88441695E-07T^2 \\ + 2.22936681E-10T^4$$

$$k(250) = 0.0157 \quad k(350) = 0.02196 \quad k(400) = 0.02461 \\ \text{std error est} = 3.3E-05 \quad \text{max error est} = 1E-04$$

250-400K

$$T(k) = 118.06 + 3008.28162k + 343663.276584k^2$$

$$T(0.0157) = 250 \quad T(0.02196) = 350 \quad T(0.02461) = 400$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 1.5$$

## BROMINE

250-350K

$$k(T) = 1.836200284 - 3.09326519E-02T + 2.07612343E-04T^2 \\ - 6.93057809E-07T^3 + 1.15148285E-09T^4 - 7.61810378E-13T^5$$

$$k(250) = 3.8E-03 \quad k(300) = 4.76E-03 \quad k(350) = 5.7E-03$$

$$\text{std error est} = 2.1E-05$$

$$\text{max error est} = 1E-04$$

Note: The pressure dependence between 250-330K has been ignored.

250-350K

$$T(k) = 63.28 + 45883.69957k + 808725.8551494k^2$$

$$T(3.8E-03) = 249 \quad T(4.76E-03) = 300 \quad T(5.7E-03) = 351$$

$$\text{std error est} = 1.6 \quad \text{max error est} = 2.5$$

270-500K

$$k(T) = 7.7275075E-02 - 8.28249983E-04T + 3.48331547E-06T^2 \\ - 5.71799839E-09T^3 + 3.50919304E-12T^4$$

$$k(270) = 0.01368 \quad k(400) = 0.02719 \quad k(500) = 0.03855$$

$$\text{std error est} = 3.7E-05$$

$$\text{max error est} = 1E-04$$

270-500K

$$T(k) = 95.54 + 15411.2231k - 219575.79653k^2 + 2403201.4742k^3$$

$$T(0.01368) = 271 \quad T(0.02719) = 401 \quad T(0.03855) = 501$$

$$\text{std error est} = 0.8 \quad \text{max error est} = 2.5$$

280-500K

$$k(T) = 3.79912E-03 - 3.38011396E-05T + 3.15886537E-07T^2 \\ - 2.25600514E-10T^3$$

$$k(280) = 0.01415 \quad k(400) = 0.02638 \quad k(500) = 0.03767$$

$$\text{std error est} = 2.5E-05$$

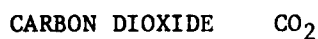
$$\text{max error est} = 1E-04$$

280-500K

$$T(k) = 128.42 + 11389.32096k - 41250.42160187k^2$$

$$T(0.01415) = 281 \quad T(0.02638) = 400 \quad T(0.03767) = 499$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 2.0$$

200-600K

$$k(T) = 2.971488E-03 - 1.33471677E-05T + 3.14443715E-07T^2 \\ - 4.75106178E-10T^3 + 2.68500151E-13T^4$$

$$k(200) = 9.51E-03 \quad k(400) = 0.02441 \quad k(600) = 0.04034$$

$$\text{std error est} = 2.2E-05$$

$$\text{max error est} = 1E-04$$

600-1000K

$$k(T) = 6.085375E-02 - 3.63680275E-04T + 1.0134366E-06T^2 \\ - 9.7042356E-10T^3 + 3.27864115E-13T^4$$

$$k(600) = 0.04036 \quad k(800) = 0.05595 \quad k(1000) = 0.06805$$

$$\text{std error est} = 5.6E-05$$

$$\text{max error est} = 1.2E-04$$

CARBON DIOXIDE (continued) 1000-1500K

$$k(T) = -4.880854E-02 + 2.05275039E-04T - 1.15912553E-07T^3 + 2.74425613E-11T^3$$

$$k(1000) = 0.0680 \quad k(1250) = 0.08027 \quad k(1500) = 0.09092$$

$$\text{std error est} = 4.9E-05 \quad \text{max error est} = 1E-04$$

200-600K

$$T(k) = 71.53 + 14079.598772k - 24697.758498k^2$$

$$T(9.51E-03) = 203 \quad T(0.02441) = 400 \quad T(0.04034) = 599$$

$$\text{std error est} = 1.1 \quad \text{max error est} = 3.5$$

600-1000K

$$T(k) = 389.988 - 335.1830848k + 137340.8296339k^2$$

$$T(0.04036) = 600 \quad T(0.05595) = 801 \quad T(0.06805) = 1003$$

$$\text{std error est} = 1.3 \quad \text{max error est} = 3.5$$

1000-1500K

$$T(k) = 438.195 - 2034.64765848k + 151207.6747921k^2$$

$$T(0.0680) = 999 \quad T(0.08027) = 1249 \quad T(0.09092) = 1503$$

$$\text{std error est} = 1.4 \quad \text{max error est} = 2.5$$

CARBON MONOXIDE CO 100-1250K

$$k(T) = -7.41704398E-04 + 9.87435265E-05T - 3.77511167E-08T^2 - 1.99334224E-11T^3 + 3.65528437E-14T^4 - 1.2427179E-17T^5$$

$$k(100) = 8.74E-03 \quad k(650) = 0.0471 \quad k(1250) = 0.07608$$

$$\text{std error est} = 4E-05 \quad \text{max error est} = 1E-04$$

100-1250K

$$T(k) = 12.162 + 8989.653527k + 97279.93110207k^2$$

$$T(8.74E-03) = 98 \quad T(0.0471) = 651 \quad T(0.07608) = 1259$$

$$\text{std error est} = 3.7 \quad \text{max error est} = 11.0$$

CARBON TETRACHLORIDE CCl<sub>4</sub> 250-500K

$$k(T) = 7.8364705E-03 - 7.3966726E-05T + 3.78688851E-07T^2 - 5.67675082E-10T^3 + 2.88855251E-13T^4$$

$$k(250) = 5.27E-03 \quad k(400) = 9.9E-03 \quad k(500) = 0.01262$$

$$\text{std error est} = 1.1E-05 \quad \text{max error est} = 1E-04$$

250-500K

$$T(k) = 108.29 + 25202.5901427k + 442601.9142055k^2$$

$$T(5.27E-03) = 253 \quad T(9.9E-03) = 401 \quad T(0.01262) = 497$$

$$\text{std error est} = 1.7 \quad \text{max error est} = 5.5$$

CHLORINE Cl<sub>2</sub> 240-700K

$$k(T) = -5.6373517E-03 + 7.42811048E-05T - 1.39215986E-07T^2 + 2.1640488E-10T^3 - 1.2881365E-13T^4$$

$$k(240) = 6.74E-03 \quad k(450) = 0.01404 \quad k(700) = 0.02144$$

$$\text{std error est} = 4.7E-05 \quad \text{max error est} = 1E-04$$

CHLORINE (continued) 240-700K  
 $T(k) = 172.043 - 13603.49935k + 5088112.16192k^2 - 265967414.84k^3$   
 $+ 5207768348.464k^4$   
 $T(6.74E-03) = 240 \quad T(0.01404) = 450 \quad T(0.02144) = 698$   
 $\text{std error est} = 1.7 \quad \text{max error est} = 5.5$

CHLORODIFLUOROMETHANE  $\text{CHClF}_2$  250-500K  
(FREON-22)  
 $k(T) = -4.0615383E-04 + 1.80841025E-05T + 6.18803419E-08T^2$   
 $k(250) = 7.98E-03 \quad k(400) = 0.01673 \quad k(500) = 0.02411$   
 $\text{std error est} = 2.4E-05 \quad \text{max error est} = 1E-04$

250-500K  
 $T(k) = 85.013 + 22663.6699172k - 228007.2338189k^2$   
 $T(7.98E-03) = 251 \quad T(0.01673) = 400 \quad T(0.02411) = 500$   
 $\text{std error est} = 0.9 \quad \text{max error est} = 2.5$

CHLOROFORM  $\text{CHCl}_3$  340-550K  
 $k(T) = -5.860675E-03 + 5.20017788E-05T - 3.8366916E-08T^2$   
 $+ 3.64052602E-11T^3$   
 $k(340) = 8.82E-03 \quad k(400) = 0.01113 \quad k(550) = 0.01719$   
 $\text{std error est} = 2.5E-05 \quad \text{max error est} = 1E-04$

340-550K  
 $T(k) = 93.34 + 29378.466083k - 162781.2342915k^2$   
 $T(8.82E-03) = 340 \quad T(0.01113) = 400 \quad T(0.01719) = 550$   
 $\text{std error est} = 0.7 \quad \text{max error est} = 1.5$

CHLOROTRIFLUOROMETHANE  $\text{CClF}_3$  250-500K  
(FREON-13)  
 $k(T) = -5.6286355E-03 + 5.68433027E-05T + 8.34249085E-09T^2$   
 $k(250) = 9.1E-03 \quad k(400) = 0.01844 \quad k(500) = 0.02488$   
 $\text{std error est} = 1.8E-05 \quad \text{max error est} = 1E-04$

250-500K  
 $T(k) = 98.24 + 16976.00664908k - 33295.38946655k^2$   
 $T(9.1E-03) = 250 \quad T(0.01844) = 400 \quad T(0.02488) = 500$   
 $\text{std error est} = 0.3 \quad \text{max error est} = 1.5$

n-DECANE  $\text{C}_{10}\text{H}_{22}$  250-500K  
 $k(T) = -5.88274E-03 + 3.72449646E-05T + 7.55109624E-08T^2$   
 $k(250) = 8.15E-03 \quad k(400) = 0.0211 \quad k(500) = 0.03162$   
 $\text{std error est} = 2.5E-05 \quad \text{max error est} = 1E-04$   
Note: Pressure dependence between 250-440K ignored.  
Note: For  $T(k)$  calculations, use the iterative procedures discussed in Section 5 and the polynomial presented above.

DEUTERIUM  $\text{D}_2$  25-400K  
 $k(T) = -5.698206E-03 + 8.4468815E-04T - 3.02792058E-06T^2$   
 $+ 1.1004468E-08T^3 - 2.1022893E-11T^4 + 1.58585846E-14T^5$

## DEUTERIUM (continued)

k(25) = 0.01369      k(250) = 0.12154      k(400) = 0.1762  
std error est = 2.2E-04      max error est = 4E-04

25-400K

 $T(k) = 0.5886 + 1513.21300425k + 4346.0399915k^2$ 

T(0.01369) = 22      T(0.12154) = 249      T(0.1762) = 402

std error est = 1.5      max error est = 2.5

DICHLORODIFLUOROMETHANE  $CCl_2F_2$  250-500K

(FREON-12)

 $k(T) = -3.233077E-03 + 3.50076218E-05T + 2.7686436E-08T^2$   
 $- 2.30654304E-12T^3$ 

k(250) = 7.21E-03      k(400) = 0.01505      k(500) = 0.0209  
std error est = 2.6E-05      max error est = 1E-04

250-500K

 $T(k) = 95.995 + 22495.971645k - 152316.4895525k^2$ 

T(7.21E-03) = 250      T(0.01505) = 400      T(0.0209) = 500

std error est = 0.5      max error est = 1.5

DICHLOROFLUOROMETHANE  $CHCl_2F$  250-450K

(FREON-21)

 $k(T) = -3.70498999E-03 + 5.72092142E-05T - 1.13430816E-07T^2$   
 $+ 1.98784186E-10T^3$ 

k(250) = 6.61E-03      k(350) = 0.01095      k(450) = 0.01718  
std error est = 3.9E-05      max error est = 1E-04

250-450K

 $T(k) = 52.34 + 34343.090676k - 655593.6727497k^2$ 

T(6.61E-03) = 251      T(0.01095) = 350      T(0.01718) = 449

std error est = 0.9      max error est = 2.0

DICHLOROTETRAFLUOROETHANE  $C_2Cl_2F_4$  250-500K

(FREON-114)

 $k(T) = 1.5549359E-02 - 7.41226495E-05T + 1.96794871E-07T^2$ 

k(250) = 9.32E-03      k(400) = 0.01739      k(500) = 0.02769  
std error est = 2.6E-05      max error est = 1E-04

250-500K

 $T(k) = -127.377 + 58481.31774k - 2155849.717k^2 + 31248863.5628k^3$ 

T(9.32E-03) = 256      T(0.01739) = 402      T(0.02769) = 502

std error est = 2.5      max error est = 6.5

ETHANE  $C_2H_6$  200-1000K
 $k(T) = -3.83815197E-02 + 5.47282126E-04T - 2.80760648E-06T^2$   
 $+ 8.74854603E-09T^3 - 1.369896E-11T^4 + 1.05765043E-14T^5$   
 $- 3.16347435E-18T^6$ 

k(200) = 0.01002      k(600) = 0.06838      k(1000) = 0.16391  
std error est = 1.9E-04      max error est = 3E-04

200-1000K

 $T(k) = 128.505 + 8110.832388k - 17342.93335k^2$ 

T(0.01002) = 208      T(0.06838) = 602      T(0.16391) = 992



ETHYL ALCOHOL     $C_2H_5OH$     250-500K

$k(T) = -2.46663E-02 + 1.5589255E-04T - 8.22954822E-08T^2$   
 $k(250) = 9.17E-03$      $k(400) = 0.02453$      $k(500) = 0.03271$   
std error est =  $2.8E-05$     max error est =  $1E-04$   
Note: Pressure dependence between 250-350K ignored.

250-500K

$T(k) = 183.774 + 6437.651482775k + 97730.4282729k^2$   
 $T(9.17E-03) = 251$      $T(0.02453) = 400$      $T(0.03271) = 499$   
std error est =  $0.7$     max error est =  $2.0$

ETHYL ETHER     $C_4H_{10}O$     250-500K

$k(T) = -7.0819597E-04 + 1.855898E-05T + 1.14117826E-07T^2$   
 $k(250) = 0.01106$      $k(400) = 0.02497$      $k(500) = 0.0371$   
std error est =  $1.8E-05$     max error est =  $1E-04$   
Note: Pressure dependence between 250-300K ignored.

250-500K

$T(k) = 106.1 + 14272.722424k - 99605.2245926k^2$   
 $T(0.01106) = 252$      $T(0.02497) = 400$      $T(0.0371) = 499$   
std error est =  $0.9$     max error est =  $2.5$

ETHYLENE     $C_2H_4$     200-450K

$k(T) = 0.1690142 - 2.71392927E-03T + 1.71636899E-05T^2$   
           $- 5.16435832E-08T^3 + 7.74044499E-11T^4 - 4.59993653E-14T^5$   
 $k(200) = 8.75E-03$      $k(350) = 0.02743$      $k(450) = 0.04262$   
std error est =  $7.0E-05$     max error est =  $1.2E-04$

200-450K

$T(k) = 108.663 + 12177.1554k - 168879.6154k^2 + 1672295.794854k^3$   
 $T(8.75E-03) = 203$      $T(0.02743) = 350$      $T(0.04262) = 450$   
std error est =  $1.3$     max error est =  $3.5$

FLUORINE     $F_2$     90-800K

$k(T) = 3.3854087E-04 + 8.27103562E-05T + 5.27622468E-08T^2$   
           $- 7.51472474E-11T^3$   
 $k(90) = 8.16E-03$      $k(400) = 0.03706$      $k(800) = 0.0618$   
std error est =  $5.9E-05$     max error est =  $1E-04$

Note: For  $T(k)$  calculations, use the iterative procedures discussed in Section 5 and the polynomial presented above.

HELIUM    He    25-300K

$k(T) = 1.028793E-02 + 8.51625139E-04T - 3.14258034E-06T^2$   
           $+ 1.02188556E-08T^3 - 1.3477236E-11T^4$   
 $k(25) = 0.02977$      $k(200) = 0.1151$      $k(300) = 0.14969$   
std error est =  $1.2E-04$     max error est =  $2E-04$

HELIUM (continued) 300-500K  
 $k(T) = -7.761491E-03 + 8.66192033E-04T - 1.5559338E-06T^2 + 1.40150565E-09T^3$   
 $k(300) = 0.1499$   $k(400) = 0.17946$   $k(500) = 0.21154$   
std error est = 1.1E-04 max error est = 2E-04

500-1500K  
 $k(T) = -9.0656E-02 + 9.37593087E-04T - 9.13347535E-07T^2 + 5.55037072E-10T^3 - 1.26457196E-13T^4$   
 $k(500) = 0.21128$   $k(1000) = 0.3622$   $k(1500) = 0.4938$   
std error est = 8.9E-04 max error est = 1.3E-03

1500-5000K  
 $k(T) = 5.26198E-02 + 3.31365073E-04T - 2.81816958E-08T^2 + 2.1409764E-12T^3$   
 $k(1500) = 0.4935$   $k(3250) = 0.9054$   $k(5000) = 1.2725$   
std error est = 2E-03 max error est = 3E-03

100-5000K  
 $T(k) = -99.57 + 2433.072575k + 1810.239628k^2 - 448.9582131k^3$   
 $T(0.1151) = 204$   $T(0.4938) = 1489$   $T(1.2725) = 5003$   
std error est = 6.5 max error est = 15.0

n-HEPTANE  $C_7H_{16}$  250-1000K  
 $k(T) = -4.606147E-02 + 5.95652224E-04T - 2.98893153E-06T^2 + 8.44612876E-09T^3 - 1.2292738E-11T^4 + 9.01270236E-15T^5 - 2.62961437E-18T^6$   
 $k(250) = 0.0082$   $k(500) = 0.0326$   $k(1000) = 0.0971$   
std error est = 1.2E-04 max error est = 4E-04  
Note: Pressure dependence between 250-370K ignored.

250-1000K  
 $T(k) = 156.21 + 12828.33732k - 81042.0901k^2 + 390630.82849k^3$   
 $T(8.2E-03) = 256$   $T(0.0326) = 502$   $T(0.0971) = 995$   
std error est = 2.9 max error est = 9.0

n-HEXANE  $C_6H_{14}$  250-1000K  
 $k(T) = 1.287757E-03 - 2.00499443E-05T + 2.37858831E-07T^2 - 1.60944555E-10T^3 + 7.71027297E-14T^4$   
 $k(250) = 8.9E-03$   $k(600) = 0.0501$   $k(1000) = 0.1353$   
std error est = 2.9E-04 max error est = 6E-04

250-1000K  
 $T(k) = 162.609 + 11501.7075k - 63679.79437k^2 + 182669.90973k^3$   
 $T(8.9E-03) = 260$   $T(0.0501) = 602$   $T(0.1353) = 1006$   
std error est = 3.5 max error est = 11.0

HYDROGEN  $H_2$  100-500K  
 $k(T) = 2.009705E-02 + 3.234622E-04T + 2.1637249E-06T^2 - 6.49151204E-09T^3 + 5.52407932E-12T^4$   
 $k(100) = 0.0681$   $k(300) = 0.1813$   $k(500) = 0.2566$

## HYDROGEN (continued)

std error est = 3.4E-04

max error est = 6E-04

500-1500K

$$k(T) = 0.1083105 + 2.21163789E-04T + 2.26380948E-07T^2 \\ - 1.74258636E-10T^3 + 4.6468625E-14T^4$$

$$k(500) = 0.2566 \quad k(1000) = 0.4281 \quad k(1500) = 0.5965$$

std error est = 3.5E-04

max error est = 7E-04

1500-2000K

$$k(T) = -0.28107269 + 1.09703479E-03T - 5.27318283E-07T^2 \\ + 1.2403865E-10T^3$$

$$k(1500) = 0.5966 \quad k(1750) = 0.6886 \quad k(2000) = 0.7960$$

std error est = 3.7E-04

max error est = 6E-04

100-500K

$$T(k) = -18.63 + 1990.8944k - 4723.849445k^2 + 19136.37907k^3$$

$$T(0.0681) = 101 \quad T(0.1813) = 301 \quad T(0.2566) = 505$$

std error est = 1.8

max error est = 5.5

500-1500K

$$T(k) = -228.573 + 2791.61736k + 187.56000746k^2$$

$$T(0.2566) = 500 \quad T(0.4281) = 1001 \quad T(0.5965) = 1503$$

std error est = 1.4

max error est = 5.0

1500-2000K

$$T(k) = -930.817 + 5242.1851374k - 1959.321732k^2$$

$$T(0.5966) = 1499 \quad T(0.6886) = 1750 \quad T(0.796) = 2001$$

std error est = 1.0

max error est = 3.0

HYDROGEN CHLORIDE HCl 200-700K

$$k(T) = 1.2288265E-04 + 3.20474254E-05T + 1.02223086E-07T^2 \\ - 1.99696412E-10T^3 + 1.16463692E-13T^4$$

$$k(200) = 9.2E-03 \quad k(400) = 0.0195 \quad k(700) = 0.0321$$

std error est = 2.8E-05

max error est = 1E-04

200-700K

$$T(k) = 61.98 + 13391.474616k + 203362.8049798k^2$$

$$T(9.2E-03) = 202 \quad T(0.0195) = 400 \quad T(0.0321) = 701$$

std error est = 1.2

max error est = 2.5

HYDROGEN IODIDE HI 250-1000K

$$k(T) = -4.35678828E-04 + 2.3083046E-05T - 3.77024198E-09T^2 \\ + 1.18389384E-12T^3$$

$$k(250) = 5.1E-03 \quad k(600) = 0.0123 \quad k(1000) = 0.0201$$

std error est = 2.7E-05

max error est = 1E-04

250-1000K

$$T(k) = 11.898 + 45338.55831k + 197725.8013557k^2$$

$$T(5.1E-03) = 248 \quad T(0.0123) = 599 \quad T(0.0201) = 1003$$

std error est = 1.4

max error est = 3.5

HYDROGEN SULFIDE  $H_2S$  220-400K

$$k(T) = -5.2404334E-03 + 6.7759251E-05T - 4.05425325E-09T^2$$

$$k(220) = 0.0095 \quad k(300) = 0.0147 \quad k(400) = 0.0212$$

$$\text{std error est} = 2.9E-05 \quad \text{max error est} = 1E-04$$

220-400K

$$T(k) = 77.82 + 14874.853457k + 14686.9999k^2$$

$$T(9.5E-03) = 220 \quad T(0.0147) = 300 \quad T(0.0212) = 400$$

$$\text{std error est} = 0.5 \quad \text{max error est} = 2.0$$

KRYPTON  $Kr$  120-700K

$$k(T) = 4.6142E-05 + 3.48571058E-05T - 1.20386082E-08T^2$$

$$k(120) = 4.06E-03 \quad k(400) = 0.01206 \quad k(700) = 0.01855$$

$$\text{std error est} = 1.7E-05 \quad \text{max error est} = 1E-04$$

120-700K

$$T(k) = 21.254 + 22220.36563k + 761572.7864265k^2$$

$$T(4.06E-03) = 124 \quad T(0.01206) = 400 \quad T(0.01855) = 696$$

$$\text{std error est} = 1.8 \quad \text{max error est} = 4.5$$

METHANE  $CH_4$  100-1000K

$$k(T) = -1.3401499E-02 + 3.6630706E-04T - 1.82248608E-06T^2$$

$$+ 5.93987998E-09T^3 - 9.1405505E-12T^4 + 6.7896889E-15T^5$$

$$- 1.95048736E-18T^6$$

$$k(100) = 0.0101 \quad k(500) = 0.067 \quad k(1000) = 0.169$$

$$\text{std error est} = 3E-04 \quad \text{max error est} = 6E-04$$

100-1000K

$$T(k) = -19.358 + 11993.5848k - 98202.38989k^2 + 631750.65118k^3$$

$$- 1542230.678766k^4$$

$$T(0.0101) = 92 \quad T(0.067) = 502 \quad T(0.169) = 994$$

$$\text{std error est} = 2.8 \quad \text{max error est} = 6.5$$

METHYL ALCOHOL  $CH_3OH$  300-550K

$$k(T) = -2.0298675E-02 + 1.21910927E-04T - 2.23748473E-08T^2$$

$$k(300) = 0.0143 \quad k(425) = 0.0275 \quad k(550) = 0.040$$

$$\text{std error est} = 3.8E-05 \quad \text{max error est} = 1E-04$$

300-550K

$$T(k) = 173.252 + 8599.676374k + 20535.0012k^2$$

$$T(0.0143) = 300 \quad T(0.0275) = 425 \quad T(0.040) = 550$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.5$$

METHYL CHLORIDE  $CH_3Cl$  250-750K

$$k(T) = -2.8950296E-03 + 2.42340563E-05T + 6.9670016E-08T^2$$

$$k(250) = 7.5E-03 \quad k(400) = 0.0179 \quad k(750) = 0.0545$$

$$\text{std error est} = 1.1E-04 \quad \text{max error est} = 2.5E-04$$

## NEON

Ne

50-500K

$$k(T) = 2.201564E-03 + 2.27517163E-04T - 2.9729466E-07T^2 + 2.08844136E-10T^3$$

$$k(50) = 0.0129 \quad k(250) = 0.0438 \quad k(500) = 0.0677$$

$$\text{std error est} = 3.4E-05 \quad \text{max error est} = 1E-04$$

500-1000K

$$k(T) = -0.0223377 + 2.83448846E-04T - 2.57636449E-07T^2 + 1.01142695E-10T^3$$

$$k(500) = 0.0676 \quad k(750) = 0.088 \quad k(1000) = 0.1046$$

$$\text{std error est} = 1.4E-04 \quad \text{max error est} = 2E-04$$

1000-5000K

$$k(T) = 0.013526582 + 1.21904517E-04T - 4.05606888E-08T^2 + 1.14406524E-11T^3 - 1.65850704E-15T^4 + 9.29114306E-20T^5$$

$$k(1000) = 0.1047 \quad k(2500) = 0.1878 \quad k(5000) = 0.2929$$

$$\text{std error est} = 2.9E-04 \quad \text{max error est} = 4E-04$$

50-500K

$$T(k) = 12.8374 + 2245.3161k + 73055.0207k^2$$

$$T(0.0129) = 54 \quad T(0.0438) = 251 \quad T(0.0677) = 500$$

$$\text{std error est} = 1.4 \quad \text{max error est} = 4$$

500-1000K

$$T(k) = 1971.304 - 65338.30244k + 844869.0777k^2 - 2954030.585k^3$$

$$T(0.0676) = 503 \quad T(0.088) = 751 \quad T(0.1046) = 1000$$

$$\text{std error est} = 2.0 \quad \text{max error est} = 5.5$$

1000-5000K

$$T(k) = -305.725 + 9215.50632k + 30228.47906k^2$$

$$T(0.1047) = 991 \quad T(0.1878) = 2491 \quad T(0.2929) = 4987$$

$$\text{std error est} = 9.0 \quad \text{max error est} = 14.5$$

## NITRIC OXIDE

NO

130-1000K

$$k(T) = 2.695164E-03 + 3.8477785E-05T + 3.79042336E-07T^2 - 1.3449086E-09T^3 + 2.15784789E-12T^4 - 1.64052333E-15T^5 + 4.79750187E-19T^6$$

$$k(130) = 0.0117 \quad k(600) = 0.0462 \quad k(1000) = 0.0724$$

$$\text{std error est} = 4.5E-05 \quad \text{max error est} = 1E-04$$

130-1000K

$$T(k) = 20.91 + 7794.64895k + 140783.3849k^2 - 857527.26795k^3$$

$$T(0.0117) = 130 \quad T(0.0462) = 597 \quad T(0.0724) = 998$$

$$\text{std error est} = 2.1 \quad \text{max error est} = 4.5$$

## NITROGEN

N<sub>2</sub>100-1500K

$$k(T) = -1.5231785E-03 + 1.18879965E-04T - 1.2092845E-07T^2 + 1.15567802E-10T^3 - 6.36537349E-14T^4 + 1.47167023E-17T^5$$

$$k(100) = 9.26E-03 \quad k(500) = 0.03861 \quad k(1500) = 0.0842$$

$$\text{std error est} = 5.2E-05 \quad \text{max error est} = 2E-04$$

## NITROGEN (continued)

1500-3500K

$$k(T) = 0.7282944 - 1.54313282E-03T + 1.3535933E-06T^2 \\ - 5.5158517E-10T^3 + 1.08449625E-13T^4 - 8.26807569E-18T^5$$

$k(1500) = 0.08382$        $k(2500) = 0.14079$        $k(3500) = 0.19131$   
 std error est = 3.2E-04      max error est = 4E-04

100-1500K

$$T(k) = 38.19 + 5560.90414k + 186184.03159k^2 - 521677.344982k^3$$

$T(9.26E-03) = 105$        $T(0.03861) = 500$        $T(0.0842) = 1515$   
 std error est = 3.5      max error est = 15.0

1500-3500K

$$T(k) = -15930.55 + 638350.15799k - 9332889.30298k^2 + 67699225.76k^3 \\ - 237257633.7266k^4 + 322622404.826k^5$$

$T(0.08382) = 1497$        $T(0.14079) = 250$        $T(0.19131) = 3497$   
 std error est = 5.5      max error est = 12.5

## NITROGEN PEROXIDE

 $NO_2$  440-640K

$$k(T) = 8.90074818 - 8.02940254E-02T + 2.89756384E-04T^2 \\ - 5.2147063E-07T^3 + 4.6839284E-10T^4 - 1.6796286E-13T^5$$

$k(440) = 0.03309$        $k(540) = 0.03752$        $k(640) = 0.04479$   
 std error est = 4.1E-05      max error est = 2E-04

440-640K

$$T(k) = -550.995 + 42497.74266k - 357393.73223k^2$$

$T(0.03309) = 464$        $T(0.03752) = 540$        $T(0.04479) = 635$   
 std error est = 7.5      max error est = 15.0

## NITROUS OXIDE

 $N_2O$ 190-1000K

$$k(T) = 6.9918875E-03 - 7.16238986E-05T + 6.16971397E-07T^2 \\ - 1.13449444E-09T^3 + 9.64569615E-13T^4 - 3.11996398E-16T^5$$

$k(200) = 9.71E-03$        $k(600) = 0.04182$        $k(1000) = 0.07042$   
 std error est = 6.8E-05      max error est = 1.2E-04

190-1000K

$$T(k) = 89.979 + 11746.9788k + 2979.32622k^2 + 193154.99479k^3$$

$T(9.71E-03) = 204$        $T(0.04182) = 601$        $T(0.07042) = 999$   
 std error est = 2.3      max error est = 5.5

## n-NONANE

 $C_9H_{20}$ 250-1000K

$$k(T) = -0.01073559242 + 7.71447107E-05T + 1.70209517E-10T^2$$

$k(250) = 8.56E-03$        $k(600) = 0.03561$        $k(1000) = 0.06658$   
 std error est = 3.0E-05      max error est = 1E-04

250-1000K

$$T(k) = 139.123 + 12954.464853k - 366.184555k^2$$

$T(8.56E-03) = 250$        $T(0.03561) = 600$        $T(0.06658) = 1000$   
 std error est = 0.4      max error est = 1.5

n-OCTANE       $C_8H_{18}$       250-500K

$k(T) = -4.0139194E-03 + 3.38796092E-05T + 8.19291819E-08T^2$   
 $k(250) = 9.58E-03$        $k(400) = 0.02265$        $k(500) = 0.03341$   
std error est =  $2.9E-05$       max error est =  $1E-04$   
Note: Pressure dependence between 250-390K ignored.

250-500K

$T(k) = 121.451 + 14436.05859k - 93780.6879k^2$   
 $T(9.58E-03) = 251$        $T(0.02265) = 400$        $T(0.03341) = 499$   
std error est =  $0.6$       max error est =  $2.5$

---

OXYGEN       $O_2$       100-1000K

$k(T) = -7.6727798E-04 + 1.03560076E-04T - 4.62034365E-08T^2$   
+  $1.51980292E-11T^3$   
 $k(100) = 9.14E-03$        $k(600) = 0.04802$        $k(1000) = 0.07179$   
std error est =  $9E-05$       max error est =  $2E-04$

1000-1500K

$k(T) = -0.18654526 + 7.05649428E-04T - 7.71025034E-07T^2$   
+  $4.02143777E-10T^3 - 7.84907953E-14T^4$   
 $k(1000) = 0.07173$        $k(1250) = 0.0846$        $k(1500) = 0.097$   
std error est =  $2E-05$       max error est =  $1E-04$

100-1000K

$T(k) = 11.465 + 9137.13572k + 65064.9850077k^2$   
 $T(9.14E-03) = 100$        $T(0.04802) = 600$        $T(0.07179) = 1003$   
std error est =  $1.2$       max error est =  $3.5$

1000-1500K

$T(k) = -212.8193 + 14703.836485k + 30477.8067k^2$   
 $T(0.07173) = 999$        $T(0.0846) = 1249$        $T(0.097) = 1500$   
std error est =  $1.0$       max error est =  $2.5$

---

n-PENTANE       $C_5H_{12}$       250-500K

$k(T) = -6.17042124E-03 + 5.06949328E-05T + 6.81013431E-08T^2$   
 $k(250) = 0.01076$        $k(375) = 0.02242$        $k(500) = 0.0362$   
std error est =  $3.2E-05$       max error est =  $1E-04$   
Note: Pressure dependence between 250-300K ignored.

250-500K

$T(k) = 120.404 + 12797.2192k - 64302.207166k^2$   
 $T(0.01076) = 251$        $T(0.02242) = 375$        $T(0.0362) = 499$   
std error est =  $0.4$       max error est =  $2.5$

---

PROPANE       $C_3H_8$       200-500K

$k(T) = -1.07682209E-02 + 8.38590352E-05T + 4.22059864E-08T^2$   
 $k(200) = 7.69E-03$        $k(350) = 0.02375$        $k(500) = 0.04171$   
std error est =  $3.6E-05$       max error est =  $1E-04$

PROPANE (continued) 200-500K  
 $T(k) = 123.418 + 10224.285427k - 28865.4345095k^2$   
 $T(7.69E-03) = 200$   $T(0.02375) = 350$   $T(0.04171) = 500$   
std error est = 0.4 max error est = 2.0

RADON  $Rn$  200-1000K  
 $k(T) = -8.228225E-05 + 1.2546552E-05T + 7.9101118E-10T^2$   
 $- 5.2693994E-12T^3 + 2.42034894E-15T^4$   
 $k(200) = 2.52E-03$   $k(600) = 6.91E-03$   $k(1000) = 0.01041$   
std error est = 1.5E-05 max error est = 1E-04

200-1000K  
 $T(k) = 37.13 + 61362.656052k + 2966201.713917k^2$   
 $T(2.52E-03) = 211$   $T(6.91E-03) = 603$   $T(0.01041) = 997$   
std error est = 2.5 max error est = 11.5

SULFUR DIOXIDE  $SO_2$  270-900K  
 $k(T) = -1.86270694E-02 + 3.19110134E-04T - 1.73644245E-06T^2$   
 $+ 5.09847985E-09T^3 - 7.53585825E-12T^4 + 5.48078289E-15T^5$   
 $- 1.56355469E-18T^6$   
 $k(270) = 8.51E-03$   $k(550) = 0.02285$   $k(900) = 0.03998$   
std error est = 1E-04 max error est = 3E-04

270-900K  
 $T(k) = 72.882 + 27366.02837k - 431142.085k^2 + 6765624.30409k^3$   
 $T(8.51E-03) = 279$   $T(0.02285) = 554$   $T(0.03998) = 910$   
std error est = 4.5 max error est = 11.5

TOLUENE  $C_7H_8$  250-600K  
 $k(T) = 5.33882E-02 - 4.90263636E-04T + 1.84066272E-06T^2$   
 $- 2.5107707E-09T^3 + 1.28558132E-12T^4$   
 $k(250) = 0.01165$   $k(450) = 0.02943$   $k(600) = 0.04615$   
std error est = 4.9E-05 max error est = 1E-04

250-600K  
 $T(k) = 49.184 + 21881.4208k - 392934.468835k^2 + 3878149.983735k^3$   
 $T(0.01165) = 257$   $T(0.02943) = 452$   $T(0.04615) = 603$   
std error est = 2.5 max error est = 8.0

TRICHLOROFLUOROMETHANE  $CCl_3F$  250-500K  
(FREON-11)  
 $k(T) = -4.57326E-03 + 4.23785103E-05T - 2.44200245E-09T^2$   
 $k(250) = 5.87E-03$   $k(400) = 0.01199$   $k(500) = 0.01601$   
std error est = 2.5E-05 max error est = 1E-04  
Note: Pressure dependence between 250-300K ignored.

250-500K  
 $T(k) = 108.8 + 23844.731142k + 37285.038633k^2$   
 $T(5.87E-03) = 250$   $T(0.01199) = 400$   $T(0.01601) = 500$   
std error est = 0.7 max error est = 1.5



TRICHLOROTRIFLUORO-  $C_2Cl_3F_3$  250-400K  
 ETHANE (FREON-113)  
 $k(T) = 6.2276996E-03 - 3.53066526E-05T + 1.33788515E-07T^2$   
 $k(250) = 5.76E-03$   $k(350) = 0.01026$   $k(400) = 0.01351$   
 std error est =  $2.1E-05$  max error est =  $1E-04$   
 Note: Pressure dependence between 250-320K ignored.  
250-400K  
 $T(k) = -22.79 + 68493.0493k - 4352430.586665k^2 + 118681269.374k^3$   
 $T(5.76E-03) = 250$   $T(0.01026) = 350$   $T(0.01351) = 401$   
 std error est = 0.6 max error est = 1.5  
 -----  
 WATER (STEAM)  $H_2O$  280-900K  
 $k(T) = -2.65056964E-02 + 3.1147143E-04T - 9.84019456E-07T^2$   
 $+ 1.92787663E-09T^3 - 1.68859732E-12T^4 + 5.48194497E-16T^5$   
 $k(280) = 0.01644$   $k(500) = 0.0358$   $k(900) = 0.078$   
 std error est =  $1.6E-04$  max error est =  $3E-04$   
280-900K  
 $T(k) = 28.726 + 17529.1632k - 157109.059k^2 + 971929.43672k^3$   
 $T(0.01644) = 279$   $T(0.0358) = 500$   $T(0.078) = 901$   
 std error est = 1.6 max error est = 3.5  
 -----  
 XENON  $Xe$  200-750K  
 $k(T) = 1.355426E-06 + 2.03984913E-05T - 5.53807454E-09T^2$   
 $k(200) = 3.86E-03$   $k(500) = 8.82E-03$   $k(750) = 0.01219$   
 std error est =  $3.9E-06$  max error est =  $1E-04$   
200-750K  
 $T(k) = 23.4897 + 40124.516223k + 1585115.24618k^2$   
 $T(3.86E-03) = 202$   $T(8.82E-03) = 501$   $T(0.01219) = 748$   
 std error est = 1.0 max error est = 2.5  
 -----

APPENDIX C  
TABLE C-I  
SUMMARY OF CONTENTS

DYNAMIC VISCOSITY ( $\times 1\text{E-}06$ ) OF  
GASEOUS ELEMENTS AND COMPOUNDS

NAME	FORMULA	APP C	PAGE
Acetone	$\text{C}_3\text{H}_6\text{O}$	C-1	
Acetylene	$\text{C}_2\text{H}_2$	C-1	
Air	-	C-1	
Ammonia	$\text{NH}_3$	C-1	
Argon	Ar	C-2	
Benzene	$\text{C}_6\text{H}_6$	C-2	
Bromine	$\text{Br}_2$	C-2	
Bromotrifluoromethane	$\text{CF}_3\text{Br}$	C-3	
iso-Butane	i- $\text{C}_4\text{H}_{10}$	C-3	
n-Butane	n- $\text{C}_4\text{H}_{10}$	C-3	
Carbon Dioxide	$\text{CO}_2$	C-3	
Carbon Monoxide	$\text{CO}$	C-3	
Carbon Tetrachloride	$\text{CCl}_4$	C-4	
Carbon Tetrafluoride	$\text{CF}_4$	C-4	
Chlorine	$\text{Cl}_2$	C-4	
Chlorodifluoromethane (FREON-22)	$\text{CHClF}_2$	C-4	
Chloroform	$\text{CHCl}_3$	C-5	
Chloropentafluoroethane	$\text{C}_2\text{ClF}_5$	C-5	
Chlorotrifluoromethane (FREON-13)	$\text{CClF}_3$	C-5	
Deuterium	$\text{D}_2$	C-5	
Dichlorodifluoromethane (FREON-12)	$\text{CCl}_2\text{F}_2$	C-5	
Dichlorofluoromethane (FREON-21)	$\text{CHCl}_2\text{F}$	C-6	
Dichlorotetrafluoroethane (FREON-114)	$\text{C}_2\text{Cl}_2\text{F}_4$	C-6	
Ethane	$\text{C}_2\text{H}_6$	C-6	
Ethyl Alcohol	$\text{C}_2\text{H}_5\text{OH}$	C-6	
Ethyl Ether	$\text{C}_4\text{H}_{10}\text{O}$	C-6	
Ethylene	$\text{C}_2\text{H}_4$	C-7	
Fluorine	$\text{F}_2$	C-7	
Helium	He	C-7	
n-Heptane	$\text{C}_7\text{H}_{16}$	C-7	
n-Hexane	$\text{C}_6\text{H}_{14}$	C-8	
Hydrogen	$\text{H}_2$	C-8	
Hydrogen Chloride	$\text{HCl}$	C-8	
Hydrogen Iodide	HI	C-9	

TABLE C-I  
(CONT.)

NAME	FORMULA	APP C PAGE
Hydrogen Sulfide	H <sub>2</sub> S	C-9
Iodine	I <sub>2</sub>	C-9
Krypton	Kr	C-9
Methane	CH <sub>4</sub>	C-10
Methyl Alcohol	CH <sub>3</sub> OH	C-10
Methyl Chloride	CH <sub>3</sub> Cl	C-10
Neon	Ne	C-10
Nitric Oxide	NO	C-11
Nitrogen	N <sub>2</sub>	C-11
Nitrogen Peroxide	NO <sub>2</sub>	C-11
Nitrous Oxide	N <sub>2</sub> O	C-11
Octafluorocyclobutane	C <sub>4</sub> F <sub>8</sub>	C-12
n-Octane	C <sub>8</sub> H <sub>18</sub>	C-12
Oxygen	O <sub>2</sub>	C-12
n-Pentane	C <sub>5</sub> H <sub>12</sub>	C-12
Propane	C <sub>3</sub> H <sub>8</sub>	C-12
Propylene	C <sub>3</sub> H <sub>6</sub>	C-13
Sulfur Dioxide	SO <sub>2</sub>	C-13
Toluene	C <sub>7</sub> H <sub>8</sub>	C-13
Trichlorofluoromethane (FREON-11)	CCl <sub>3</sub> F	C-13
Trichlorotrifluoroethane (FREON-113)	C <sub>2</sub> Cl <sub>3</sub> F <sub>3</sub>	C-13
Trifluoromethane	CHF <sub>3</sub>	C-14
Water	H <sub>2</sub> O	C-14
Xenon	Xe	C-14

# APPENDIX C FORMAT EXAMPLE

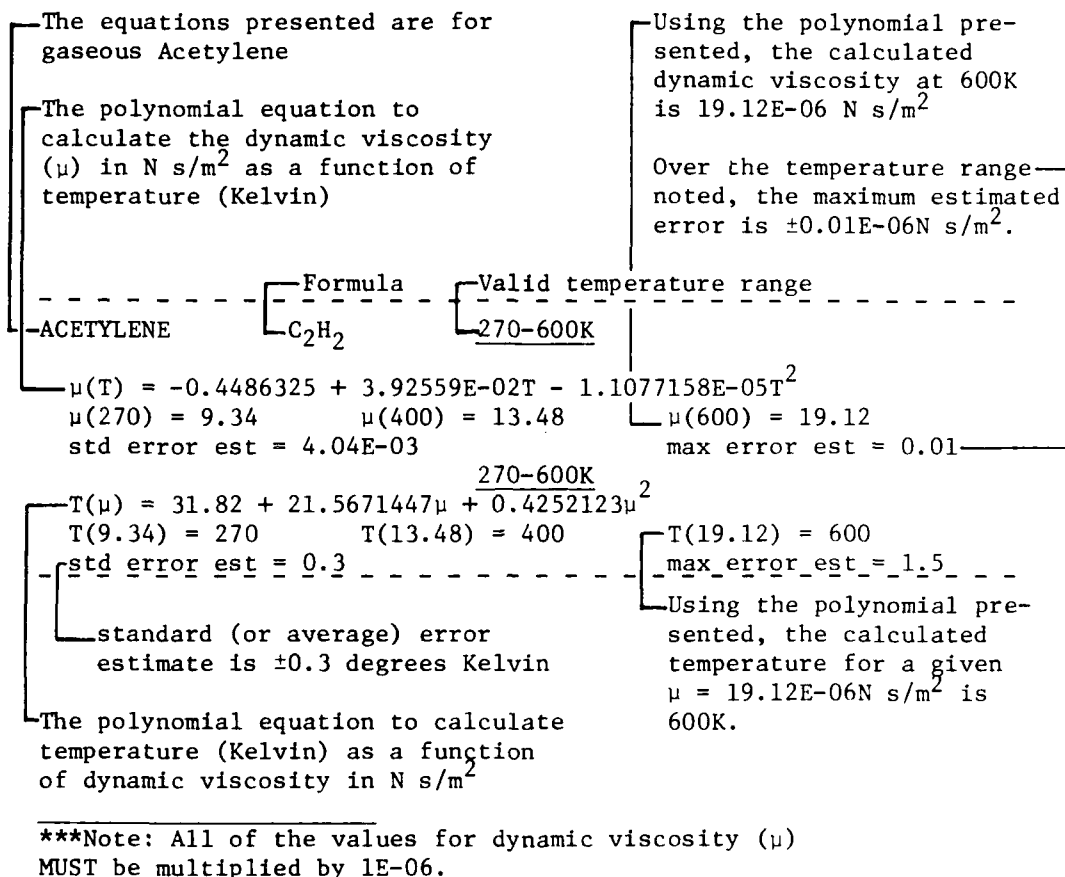


FIGURE C-1

# APPENDIX C

## DYNAMIC VISCOSITY ( $\times 1E-06$ ) OF GASEOUS ELEMENTS AND COMPOUNDS

-----  
ACETONE       $C_3H_6O$       250-650K

$$\mu(T) = 3.996401 + 1.51018819E-03T + 4.44247E-05T^2 - 2.47973E-08T^3$$

$\mu(250) = 6.76$        $\mu(400) = 10.12$        $\mu(650) = 16.94$   
std error est =  $1.906E-02$       max error est = 0.04

250-650K

$$T(\mu) = -191.27 + 84.748208\mu - 3.388215\mu^2 + 7.7871645E-02\mu^3$$

$T(6.76) = 251$        $T(10.12) = 400$        $T(16.94) = 651$   
std error est = 0.9      max error est = 2

-----  
ACETYLENE       $C_2H_2$       270-600K

$$\mu(T) = -0.4486325 + 3.92559E-02T - 1.1077158E-05T^2$$

$\mu(270) = 9.34$        $\mu(400) = 13.48$        $\mu(600) = 19.12$   
std error est =  $4.04E-03$       max error est = 0.01

270-600K

$$T(\mu) = 31.82 + 21.5671447\mu + .42521234\mu^2$$

$T(9.34) = 270$        $T(13.48) = 400$        $T(19.12) = 600$   
std error est = 0.3      max error est = 1.5

-----  
AIR      80-600K

$$\mu(T) = -0.98601 + 0.09080125T - 1.17635575E-04T^2 + 1.2349703E-07T^3$$

$\mu(80) = 5.59$        $\mu(350) = 20.81$        $\mu(600) = 30.31$   
std error est =  $1.47E-02$       max error est = 0.07

600-2000K

$$\mu(T) = 4.8856745 + 5.43232E-02T - 2.4261775E-05T^2 + 7.9306E-09T^3$$

$\mu(600) = 30.32$        $\mu(1200) = 46.55$        $\mu(2000) = 62.27$   
std error est =  $1.98E-02$       max error est = 0.05

80-600K

$$T(\mu) = 23.211 + 8.59256\mu + 0.342764\mu^2$$

$T(5.59) = 82$        $T(20.81) = 350$        $T(30.31) = 600$   
std error est = 0.7      max error est = 1.5

600-2000K

$$T(\mu) = 92.81 + 3.601092\mu + 0.43380968\mu^2$$

$T(30.32) = 601$        $T(46.55) = 1200$        $T(62.27) = 1999$   
std error est = 1.0      max error est = 2.5

-----  
AMMONIA       $NH_3$       200-1000K

$$\mu(T) = 0.3639 + 2.999278E-02T + 1.25282E-05T^2 - 7.033645E-09T^3$$

$\mu(200) = 6.81$        $\mu(600) = 21.35$        $\mu(1000) = 35.85$   
std error est =  $3.57E-02$       max error est = 0.08

AMMONIA (continued) 200-1000K  
 $\mu(T) = 20.22 + 27.09159\mu + 2.94502348E-03\mu^2$   
 $T(6.81) = 205$   $T(21.35) = 600$   $T(35.85) = 995$   
 - std error est = 2.2 - - - - - max error est = 5.0

ARGON Ar 60-540K  
 $\mu(T) = 1.22573 + 5.9456964E-02T + 1.897011E-04T^2 - 8.171242E-07T^3$   
 $+ 1.2939183E-09T^4 - 7.5027442E-13T^5$   
 $\mu(60) = 5.32$   $\mu(350) = 25.72$   $\mu(540) = 35.55$   
 std error est = 1.95E-02 max error est = 0.03

540-2200K  
 $\mu(T) = 4.03764 + 7.3665688E-02T - 3.3867E-05T^2 + 1.127158E-08T^3$   
 $- 1.585569E-12T^4$   
 $\mu(540) = 35.58$   $\mu(1250) = 61.35$   $\mu(2200) = 85.06$   
 std error est = 0.03 max error est = 0.05

60-540K  
 $T(\mu) = 12.722 + 9.0267675\mu + 0.161221378\mu^2$   
 $T(5.32) = 65$   $T(25.72) = 351$   $T(35.55) = 537$   
 std error est = 1.7 max error est = 5.0

540-2200K  
 $T(\mu) = 108.244 + 3.305827\mu + 0.24958985\mu^2$   
 $T(35.58) = 542$   $T(61.35) = 1250$   $T(85.06) = 2195$   
 - std error est = 1.1 - - - - - max error est = 5.0

BENZENE  $C_6H_6$  270-650K  
 $\mu(T) = 0.39324 + 2.24768E-02T + 8.090553E-06T^2 - 7.8349307E-09T^3$   
 $\mu(270) = 6.90$   $\mu(400) = 10.18$   $\mu(650) = 16.27$   
 std error est = 0.02 max error est = 0.04

270-650K  
 $T(\mu) = 12.343 + 36.249\mu + 0.177428\mu^2$   
 $T(6.90) = 272$   $T(10.18) = 400$   $T(16.27) = 649$   
 - std error est = 0.9 - - - - - max error est = 2.0

BORON TRIFLUORIDE  $BF_3$  190-700K  
 $\mu(T) = 1.401165 + 5.644982E-02T - 1.4088857E-05T^2$   
 $\mu(190) = 11.62$   $\mu(400) = 21.73$   $\mu(700) = 34.01$   
 std error est = 1.9E-02 max error est = 0.03

190-700K  
 $T(\mu) = -38.33 + 19.737077\mu - 0.0468724\mu^2 + 3.08592457E-03\mu^3$   
 $T(11.62) = 190$   $T(21.73) = 400$   $T(34.01) = 700$   
 - std error est = 0.5 - - - - - max error est = 1.5

BROMINE  $Br_2$  280-800K  
 $\mu(T) = 0.8027126 + 4.9413942E-02T - 1.70534854E-06T^2$   
 $\mu(280) = 14.50$   $\mu(500) = 25.08$   $\mu(800) = 39.24$   
 std error est = 4.35E-02 max error est = 0.21

BROMINE (continued) 280-800K

$$\mu(T) = -51.3 + 24.52145\mu - 0.153459363\mu^2 + 2.0985285E-03\mu^3$$

$$T(14.50) = 278 \quad T(25.08) = 500 \quad T(39.24) = 801$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 1.5$$

BROMOTRIFLUOROMETHANE  $\text{CF}_3\text{Br}$  230-500K

$$\mu(T) = -1.62177 + 0.0694797T - 4.550649E-05T^2 + 2.0833526E-08T^3$$

$$\mu(230) = 12.20 \quad \mu(350) = 18.01 \quad \mu(500) = 24.35$$

$$\text{std error est} = 0.02 \quad \text{max error est} = 0.09$$

$$T(\mu) = 33.415 + 13.0473238\mu + 0.25127636\mu^2$$

$$T(12.20) = 230 \quad T(18.01) = 350 \quad T(24.35) = 500$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.5$$

iso-BUTANE  $\text{i-C}_4\text{H}_{10}$  270-520K

$$\mu(T) = -0.102505 + 2.6972076E-02T - 4.2918193E-06T^2$$

$$\mu(270) = 6.87 \quad \mu(400) = 10.00 \quad \mu(520) = 12.76$$

$$\text{std error est} = 6.5E-03 \quad \text{max error est} = 0.02$$

$$T(\mu) = 7.628 + 35.967103\mu + 0.3272017\mu^2$$

$$T(6.87) = 270 \quad T(10.00) = 400 \quad T(12.76) = 520$$

$$\text{std error est} = 0.3 \quad \text{max error est} = 1.5$$

n-BUTANE  $\text{n-C}_4\text{H}_{10}$  270-520K

$$\mu(T) = -0.01099487 + 2.634504E-02T - 3.54700854E-06T^2$$

$$\mu(270) = 6.84 \quad \mu(400) = 9.96 \quad \mu(520) = 12.73$$

$$\text{std error est} = 5.9E-03 \quad \text{max error est} = 0.02$$

$$T(\mu) = 3.12 + 37.1408242\mu + 0.271992359\mu^2$$

$$T(6.84) = 270 \quad T(9.96) = 400 \quad T(12.73) = 520$$

$$\text{std error est} = 0.3 \quad \text{max error est} = 1.5$$

CARBON DIOXIDE  $\text{CO}_2$  170-2000K

$$\mu(T) = -0.8095191 + 6.0395329E-02T - 2.824853E-05T^2 + 9.843776E-09T^3 - 1.47315277E-12T^4$$

$$\mu(170) = 8.69 \quad \mu(1100) = 42.39 \quad \mu(2000) = 62.17$$

$$\text{std error est} = 3E-02 \quad \text{max error est} = 0.1$$

$$T(\mu) = 25.166 + 15.2582\mu + 0.1780093719\mu^2 + 1.4129E-03\mu^3$$

$$T(8.69) = 172 \quad T(42.39) = 1099 \quad T(62.17) = 2001$$

$$\text{std error est} = 1.3 \quad \text{max error est} = 5.0$$

CARBON MONOXIDE  $\text{CO}$  80-1500K

$$\mu(T) = -0.524575 + 7.9606E-02T - 7.82295E-05T^2 + 6.2821488E-08T^3 - 2.83747E-11T^4 + 5.317831E-15T^5$$

$$\mu(80) = 5.37 \quad \mu(800) = 35.38 \quad \mu(1500) = 51.63$$

## CARBON MONOXIDE (continued)

std error est = 2.62E-02

max error est = 0.03

80-1500K

$$T(\mu) = 21.08 + 10.0217\mu + 0.289517\mu^2 + 1.4002864E-03\mu^3$$

$$T(5.37) = 83$$

$$T(35.38) = 800$$

$$T(51.63) = 1503$$

$$\text{std error est} = 1.3$$

$$\text{max error est} = 3.5$$

CARBON TETRACHLORIDE  $\text{CCl}_4$  280-800K

$$\mu(T) = -1.5110416 + 4.3798388E-02T - 2.02626E-05T^2 + 6.144E-09T^3$$

$$\mu(280) = 9.30$$

$$\mu(550) = 17.47$$

$$\mu(800) = 23.71$$

$$\text{std error est} = 2.2E-02$$

$$\text{max error est} = 0.04$$

280-800K

$$T(\mu) = 53.258 + 19.890474\mu + 0.489386918\mu^2$$

$$T(9.30) = 281$$

$$T(17.47) = 550$$

$$T(23.71) = 800$$

$$\text{std error est} = 0.9$$

$$\text{max error est} = 2.5$$

CARBON TETRAFLUORIDE  $\text{CF}_4$  230-500K

$$\mu(T) = -1.235676 + 7.815327E-02T - 6.115548E-05T^2 + 2.95168E-08T^3$$

$$\mu(230) = 13.86$$

$$\mu(400) = 22.13$$

$$\mu(500) = 26.24$$

$$\text{std error est} = 2.7E-03$$

$$\text{max error est} = 0.01$$

230-500K

$$T(\mu) = 37.74 + 9.70199\mu + 0.30144808\mu^2$$

$$T(13.86) = 230$$

$$T(22.13) = 400$$

$$T(26.24) = 500$$

$$\text{std error est} = 0.1$$

$$\text{max error est} = 1.0$$

CHLORINE  $\text{Cl}_2$  270-800K

$$\mu(T) = -1.81447 + 5.814046E-02T - 2.299287E-05T^2 + 5.015775E-09T^3$$

$$\mu(270) = 12.31$$

$$\mu(550) = 24.04$$

$$\mu(800) = 32.55$$

$$\text{std error est} = 0.08$$

$$\text{max error est} = 0.15$$

270-800K

$$T(\mu) = 56.456 + 14.237878\mu + 0.262332581\mu^2$$

$$T(12.31) = 271$$

$$T(24.04) = 550$$

$$T(32.55) = 798$$

$$\text{std error est} = 2.5$$

$$\text{max error est} = 5.0$$

CHLORODIFLUOROMETHANE  $\text{CHClF}_2$  250-500K

(FREON-22)

$$\mu(T) = -0.7369597 + 4.9394676E-02T - 1.2112332E-05T^2$$

$$\mu(250) = 10.85$$

$$\mu(400) = 17.08$$

$$\mu(500) = 20.93$$

$$\text{std error est} = 0.02$$

$$\text{max error est} = 0.03$$

250-500K

$$T(\mu) = 23.086 + 18.911\mu + 0.18471282\mu^2$$

$$T(10.85) = 250$$

$$T(17.08) = 400$$

$$T(20.93) = 500$$

$$\text{std error est} = 0.3$$

$$\text{max error est} = 2.0$$



CHLOROFORM  $\text{CHCl}_3$  250-650K

$$\mu(T) = -0.389489 + 3.6808\text{E-}02T - 2.72048\text{E-}06T^2 - 3.194456\text{E-}09T^3$$

$\mu(250) = 8.59$        $\mu(450) = 15.33$        $\mu(650) = 21.51$   
 std error est = 0.022      max error est = 0.09

250-650K

$$T(\mu) = 23.48 + 24.644568\mu + 0.207098\mu^2$$

$T(8.59) = 250$        $T(15.33) = 450$        $T(21.51) = 649$   
 - std error est = 0.8 - - - - - max error est = 3.5

CHLOROPENTAFLUOROETHANE  $\text{C}_2\text{ClF}_5$  250-500K

$$\mu(T) = 0.357912 + 4.440886\text{E-}02T - 1.014652\text{E-}05T^2$$

$\mu(250) = 10.83$        $\mu(400) = 16.50$        $\mu(500) = 20.03$   
 std error est = 3.5E-03      max error est = 0.01

250-500K

$$T(\mu) = 0.2646 + 20.875165\mu + 0.203445135\mu^2$$

$T(10.83) = 250$        $T(16.50) = 400$        $T(20.03) = 500$   
 - std error est = 0.2 - - - - - max error est = 1.0

CHLOROTRIFLUOROMETHANE  $\text{CClF}_3$  230-500K

(FREON-13)

$$\mu(T) = 4.018574 + 2.3020865\text{E-}02T + 5.190552\text{E-}05T^2 - 4.09445\text{E-}08T^3$$

$\mu(230) = 11.56$        $\mu(400) = 18.91$        $\mu(500) = 23.39$   
 std error est = 4.4E-03      max error est = 0.01

230-500K

$$T(\mu) = -53.645 + 25.566055\mu - 8.24565722\text{E-}02\mu^2$$

$T(11.56) = 231$        $T(18.91) = 400$        $T(23.39) = 499$   
 - std error est = 0.5 - - - - - max error est = 2.5

DEUTERIUM  $\text{D}_2$  15-500K

$$\mu(T) = -0.0374066 + 0.07422285T - 1.98491852\text{E-}04T^2 + 4.0366\text{E-}07T^3 - 3.18855544\text{E-}10T^4$$

$\mu(15) = 1.03$        $\mu(300) = 12.68$        $\mu(500) = 17.98$   
 std error est = 4.5E-02      max error est = 0.09

15-500K

$$T(\mu) = -0.449 + 13.1729602\mu + 0.8102567096\mu^2$$

$T(1.03) = 14$        $T(12.68) = 297$        $T(17.98) = 498$   
 - std error est = 1.6 - - - - - max error est = 4.5

DICHLORODIFLUOROMETHANE  $\text{CCl}_2\text{F}_2$  250-500K

(FREON-12)

$$\mu(T) = -0.904423 + 5.03878\text{E-}02T - 1.7884615\text{E-}05T^2$$

$\mu(250) = 10.57$        $\mu(400) = 16.39$        $\mu(500) = 19.82$   
 std error est = 5.3E-03      max error est = 0.01

DICHLORODIFLUOROMETHANE (continued) 250-500K

$$T(\mu) = 38.998 + 16.2507676\mu + 0.3528873\mu^2$$

$$T(10.57) = 250 \quad T(16.39) = 400 \quad T(19.82) = 500$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.5$$

DICHLOROFLUOROMETHANE  $\text{CHCl}_2\text{F}$  280-500K

(FREON-21)

$$\mu(T) = 0.033118573 + 4.03724167\text{E-}02T - 5.7792208\text{E-}06T^2$$

$$\mu(280) = 10.88 \quad \mu(400) = 15.26 \quad \mu(500) = 18.77$$

$$\text{std error est} = 5.8\text{E-}03 \quad \text{max error est} = 0.01$$

280-500K

$$T(\mu) = 2.23 + 24.1579854\mu + 0.1253726\mu^2$$

$$T(10.88) = 280 \quad T(15.26) = 400 \quad T(18.77) = 500$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.5$$

DICHLOROTETRAFLUOROETHANE  $\text{C}_2\text{Cl}_2\text{F}_4$  230-500K

(FREON-114)

$$\mu(T) = 4.649332 + 9.784407\text{E-}03T + 5.818667\text{E-}05T^2 - 4.542242\text{E-}08T^3$$

$$\mu(230) = 9.43 \quad \mu(400) = 14.97 \quad \mu(500) = 18.41$$

$$\text{std error est} = 6.2\text{E-}03 \quad \text{max error est} = 0.01$$

230-500K

$$T(\mu) = -87.64 + 35.9444125\mu - 0.2222265\mu^2$$

$$T(9.43) = 232 \quad T(14.97) = 401 \quad T(18.41) = 499$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 2.5$$

ETHANE  $\text{C}_2\text{H}_6$  190-1000K

$$\mu(T) = -0.5107728 + 3.76582\text{E-}02T - 1.59412113\text{E-}05T^2 + 3.906\text{E-}09T^3$$

$$\mu(190) = 6.10 \quad \mu(600) = 17.19 \quad \mu(1000) = 25.11$$

$$\text{std error est} = 3.3\text{E-}02 \quad \text{max error est} = 0.03$$

190-1000K

$$T(\mu) = 43.829 + 20.323073\mu + 0.7026353\mu^2$$

$$T(6.10) = 194 \quad T(17.19) = 601 \quad T(25.11) = 997$$

$$\text{std error est} = 2.2 \quad \text{max error est} = 4.5$$

ETHYL ALCOHOL  $\text{C}_2\text{H}_5\text{OH}$  270-600K

$$\mu(T) = -0.0633595 + 3.2071347\text{E-}02T - 6.25079576\text{E-}06T^2$$

$$\mu(270) = 8.14 \quad \mu(400) = 11.77 \quad \mu(600) = 16.93$$

$$\text{std error est} = 3.9\text{E-}03 \quad \text{max error est} = 0.01$$

270-600K

$$T(\mu) = 10.415 + 29.22028895\mu + 0.330513733\mu^2$$

$$T(8.14) = 270 \quad T(11.77) = 400 \quad T(16.93) = 600$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 1.5$$

ETHYL ETHER  $\text{C}_4\text{H}_{10}\text{O}$  250-650K

$$\mu(T) = -0.82017 + 2.98341946\text{E-}02T - 4.938627\text{E-}06T^2 - 2.82999\text{E-}09T^3$$

$$\mu(250) = 6.29 \quad \mu(450) = 11.35 \quad \mu(650) = 15.71$$

ETHYL ETHER (continued)

std error est = 0.02

max error est = 0.03

250-650K

$$T(\mu) = 51.2 + 27.634314\mu + 0.6622779\mu^2$$

$$T(6.29) = 251$$

$$T(11.35) = 450$$

$$T(15.71) = 649$$

$$\text{std error est} = 0.9$$

$$\text{max error est} = 3.5$$

ETHYLENE



190-1500K

$$\mu(T) = -0.3919492 + 0.040557T - 1.6439973E-05T^2 + 3.7310454E-09T^3$$

$$\mu(190) = 6.75$$

$$\mu(800) = 23.44$$

$$\mu(1500) = 36.05$$

$$\text{std error est} = 2.6E-02$$

$$\text{max error est} = 0.05$$

190-1500K

$$T(\mu) = 23.3 + 22.4670445\mu + 0.34307964\mu^2 + 4.8478305E-03\mu^3$$

$$T(6.75) = 192$$

$$T(23.44) = 801$$

$$T(36.05) = 1506$$

$$\text{std error est} = 1.1$$

$$\text{max error est} = 6.5$$

FLUORINE



90-500K

$$\mu(T) = -1.3474535 + 0.1088684T - 1.032287E-04T^2 + 6.02076E-08T^3$$

$$\mu(90) = 7.66$$

$$\mu(350) = 26.69$$

$$\mu(500) = 34.81$$

$$\text{std error est} = 3E-02$$

$$\text{max error est} = 0.1$$

90-500K

$$T(\mu) = 23.06 + 7.555066\mu + 0.176432568\mu^2$$

$$T(7.66) = 91$$

$$T(26.69) = 350$$

$$T(34.81) = 500$$

$$\text{std error est} = 0.7$$

$$\text{max error est} = 2.5$$

HELIUM



1-500K

$$\mu(T) = 0.39414 + 0.17213335T - 1.38733E-03T^2 + 8.020045E-06T^3 - 2.4278655E-08T^4 + 3.641644E-11T^5 - 2.14117E-14T^6$$

$$\mu(1) = 0.56$$

$$\mu(250) = 17.53$$

$$\mu(500) = 28.17$$

$$\text{std error est} = 9.2E-02$$

$$\text{max error est} = 0.19$$

500-2500K

$$\mu(T) = 7.442412 + 4.6649873E-02T - 1.0385665E-05T^2 + 1.35269E-09T^3$$

$$\mu(500) = 28.34$$

$$\mu(1500) = 58.61$$

$$\mu(2500) = 80.29$$

$$\text{std error est} = 4E-02$$

$$\text{max error est} = 0.09$$

1-500K

$$T(\mu) = -2.78 + 4.7805365\mu + 0.702059\mu^2 - 8.7384854E-03\mu^3$$

$$T(.56) = 0$$

$$T(17.53) = 250$$

$$T(28.17) = 494$$

$$\text{std error est} = 2.2$$

$$\text{max error est} = 7.0$$

500-2500K

$$T(\mu) = -15.4944 + 11.26614\mu + 0.249906096\mu^2$$

$$T(28.34) = 505$$

$$T(58.61) = 1503$$

$$T(80.29) = 2500$$

$$\text{std error est} = 1.9$$

$$\text{max error est} = 5.5$$

n-HEPTANE



270-580K

n-HEPTANE (continued) 270-580K  
 $\mu(T) = 1.540097 + 1.095157E-02T + 1.800664E-05T^2 - 1.36379E-08T^3$   
 $\mu(270) = 5.54$   $\mu(400) = 7.93$   $\mu(580) = 11.29$   
std error est = 3.1E-03 max error est = 0.01

270-580K  
 $T(\mu) = -31.9 + 55.191463\mu - 9.495688E-02\mu^2$   
 $T(5.54) = 271$   $T(7.93) = 400$   $T(11.29) = 579$   
std error est = 0.6 max error est = 1.5

n-HEXANE  $C_6H_{14}$  270-900K  
 $\mu(T) = 1.545412 + 1.150809E-02T + 2.722165E-05T^2 - 3.269E-08T^3$   
 $+ 1.245459E-11T^4$   
 $\mu(270) = 6.06$   $\mu(600) = 12.80$   $\mu(900) = 18.29$   
std error est = 4.6E-03 max error est = 0.01

270-900K  
 $T(\mu) = -35.27 + 53.9008\mu - 0.760933\mu^2 + 3.349925E-02\mu^3$   
 $T(6.06) = 271$   $T(12.80) = 600$   $T(18.29) = 901$   
std error est = 0.5 max error est = 2.0

HYDROGEN  $H_2$  10-500K  
 $\mu(T) = -0.135666 + 6.84115878E-02T - 3.928747E-04T^2 + 1.8996E-06T^3$   
 $- 5.23104E-09T^4 + 7.4490972E-12T^5 - 4.250937E-15T^6$   
 $\mu(10) = 0.51$   $\mu(250) = 7.90$   $\mu(500) = 12.72$   
std error est = 9.6E-03 max error est = 0.03

500-2000K  
 $\mu(T) = 2.72941 + 2.3224377E-02T - 7.6287854E-06T^2 + 2.92585E-09T^3$   
 $- 5.2889938E-13T^4$   
 $\mu(500) = 12.77$   $\mu(1250) = 24.26$   $\mu(2000) = 33.61$   
std error est = 3.3E-02 max error est = 0.05

10-500K  
 $T(\mu) = -7.126 + 19.551451\mu + 1.6191086\mu^2$   
 $T(0.51) = 3$   $T(7.90) = 248$   $T(12.72) = 503$   
std error est = 2.9 max error est = 7.0

500-2000K  
 $T(\mu) = -116.25 + 39.399135\mu + 0.69646657\mu^2$   
 $T(12.77) = 500$   $T(24.26) = 1249$   $T(33.61) = 1995$   
std error est = 2.5 max error est = 6.0

HYDROGEN CHLORIDE  $HCl$  250-650K  
 $(T) = -10.37895 + 0.146304667T - 3.3750673E-04T^2 + 5.204805E-07T^3$   
 $- 3.066023E-10T^4$   
 $(250) = 12.04$   $(450) = 21.97$   $(650) = 30.33$   
std error est = 0.143 max error est = 0.25

HYDROGEN CHLORIDE (continued) 250-650K

$$T(\mu) = 54.8 + 14.15333\mu + 0.17335227\mu^2$$

$$T(12.04) = 250$$

$$T(21.97) = 449$$

$$T(30.33) = 644$$

$$\text{std error est} = 3.9$$

$$\text{max error est} = 7.5$$

HYDROGEN IODIDE HI 250-650K

$$\mu(T) = -0.8210072 + 6.96502E-02T - 1.1987247E-05T^2$$

$$\mu(250) = 15.84$$

$$\mu(400) = 25.12$$

$$\mu(650) = 39.39$$

$$\text{std error est} = 2.6E-02$$

$$\text{max error est} = 0.09$$

$$T(\mu) = 18.0 + 13.73048\mu + 5.8615567E-02\mu^2$$

$$T(15.84) = 250$$

$$T(25.12) = 400$$

$$T(39.39) = 650$$

$$\text{std error est} = 0.6$$

$$\text{max error est} = 2.0$$

HYDROGEN SULFIDE H<sub>2</sub>S 270-500K

$$\mu(T) = -1.880078 + 5.29022575E-02T - 1.49125874E-05T^2$$

$$\mu(270) = 11.32$$

$$\mu(400) = 16.89$$

$$\mu(500) = 20.84$$

$$\text{std error est} = 1.6E-02$$

$$\text{max error est} = 0.03$$

$$T(\mu) = 46.59 + 17.386465\mu + 0.2091804\mu^2$$

$$T(11.32) = 270$$

$$T(16.89) = 400$$

$$T(20.84) = 500$$

$$\text{std error est} = 0.5$$

$$\text{max error est} = 1.5$$

IODINE I<sub>2</sub> 370-700K

$$\mu(T) = -9.77787 + 0.12652959T - 2.34192527E-04T^2 + 2.94743E-07T^3 - 1.409635E-10T^4$$

$$\mu(370) = 17.26$$

$$\mu(550) = 25.11$$

$$\mu(700) = 31.29$$

$$\text{std error est} = 4E-02$$

$$\text{max error est} = 0.04$$

$$T(\mu) = 11.76 + 19.2390557\mu + 8.7220577E-02\mu^2$$

$$T(17.26) = 370$$

$$T(25.11) = 550$$

$$T(31.29) = 699$$

$$\text{std error est} = 0.9$$

$$\text{max error est} = 2.5$$

KRYPTON Kr 100-1500K

$$\mu(T) = -0.465233 + 9.9000315E-02T - 4.278998E-05T^2 + 1.9612E-09T^3 + 1.0362237E-11T^4 - 3.592904E-15T^5$$

$$\mu(100) = 9.01$$

$$\mu(800) = 55.42$$

$$\mu(1500) = 83.55$$

$$\text{std error est} = 5.5E-02$$

$$\text{max error est} = 0.3$$

$$T(\mu) = 15.03 + 9.1084\mu + 6.7458509E-02\mu^2 + 4.33414E-04\mu^3$$

$$T(9.01) = 103$$

$$T(55.42) = 801$$

$$T(83.55) = 1500$$

$$\text{std error est} = 1.3$$

$$\text{max error est} = 6.5$$

METHANE CH<sub>4</sub> 70-1000K

$$\mu(T) = 0.2968267 + 3.711201E-02T + 1.218298E-05T^2 - 7.02426E-08T^3 + 7.543269E-11T^4 - 2.7237166E-14T^5$$

$\mu(70) = 2.93$   $\mu(550) = 18.24$   $\mu(1000) = 27.54$   
std error est = 3E-02 max error est = 0.09

70-1000K

$$T(\mu) = 2.184 + 23.32102\mu + 0.179160065\mu^2 + 1.0455235E-02\mu^3$$

$T(2.93) = 72$   $T(18.24) = 551$   $T(27.54) = 999$   
std error est = 1.4 max error est = 3.5

METHYL ALCOHOL CH<sub>3</sub>OH 250-650K

$$\mu(T) = 1.1979 + 0.0245028T + 1.8616274E-05T^2 - 1.3067482E-08T^3$$

$\mu(250) = 8.28$   $\mu(400) = 13.14$   $\mu(650) = 21.40$   
std error est = 3.2E-02 max error est = 0.04

250-650K

$$T(\mu) = -4.983 + 31.162925\mu - 2.8760994E-02\mu^2$$

$T(8.28) = 251$   $T(13.14) = 400$   $T(21.40) = 649$   
std error est = 1.1 max error est = 2.5

METHYL CHLORIDE CH<sub>3</sub>Cl 250-660K

$$\mu(T) = 0.282322 + 0.0364907T - 2.48976E-06T^2$$

$\mu(250) = 9.25$   $\mu(400) = 14.48$   $\mu(660) = 23.28$   
std error est = 2.4E-02 max error est = 0.04

250-660K

$$T(\mu) = -6.86 + 27.202172\mu + 6.180147E-02\mu^2$$

$T(9.25) = 250$   $T(14.48) = 400$   $T(23.28) = 660$   
std error est = 0.7 max error est = 2.0

NEON Ne 20-450K

$$\mu(T) = -0.261473 + 0.2007328T - 7.54726E-04T^2 + 2.5795522E-06T^3 - 4.7146844E-09T^4 + 3.3937307E-12T^5$$

$\mu(20) = 3.47$   $\mu(250) = 27.95$   $\mu(450) = 41.59$   
std error est = 4E-02 max error est = 0.09

450-1200K

$$\mu(T) = 9.5675148 + 8.4038686E-02T - 3.2087447E-05T^2 + 7.366716E-09T^3$$

$\mu(450) = 41.56$   $\mu(850) = 62.34$   $\mu(1200) = 76.94$   
std error est = 2.9E-02 max error est = 0.06

20-450K

$$T(\mu) = 0.08 + 4.9693056\mu + 0.141318424\mu^2$$

$T(3.47) = 19$   $T(27.95) = 249$   $T(41.59) = 451$   
std error est = 0.5 max error est = 2.5

NEON (continued) 450-1200K  
 $T(\mu) = -1.85 + 5.337484\mu + 0.1336294\mu^2$   
 $T(41.56) = 451$   $T(62.34) = 850$   $T(76.94) = 1200$   
 - std error est = 0.6 - - - - - max error est = 2.0 -

NITRIC OXIDE NO 110-1500K  
 $\mu(T) = -0.80134 + 8.61223E-02T - 8.053232E-05T^2 + 6.3144787E-08T^3$   
 $- 2.8327E-11T^4 + 5.325217E-15T^5$   
 $\mu(110) = 7.78$   $\mu(800) = 39.03$   $\mu(1500) = 57.33$   
 std error est = 2.6E-02 max error est = 0.06  
110-1500K  
 $T(\mu) = 22.84 + 9.70756\mu + 0.2197071\mu^2 + 1.0689525E-03\mu^3$   
 $T(7.78) = 112$   $T(39.03) = 800$   $T(57.33) = 1503$   
 - std error est = 1.1 - - - - - max error est = 3.5 -

NITROGEN  $N_2$  80-2200K  
 $\mu(T) = 0.025465 + 7.5336535E-02T - 6.51566245E-05T^2 + 4.34945E-08T^3$   
 $- 1.5622457E-11T^4 + 2.249666E-15T^5$   
 $\mu(80) = 5.66$   $\mu(1250) = 46.06$   $\mu(2200) = 63.51$   
 std error est = 3.9E-02 max error est = 0.11  
80-2200K  
 $T(\mu) = 23.03 + 9.279727\mu + 0.3237956\mu^2 + 1.14361184E-03\mu^3$   
 $T(5.66) = 86$   $T(46.06) = 1249$   $T(63.51) = 2211$   
 - std error est = 1.5 - - - - - max error est = 11.0 -

NITROGEN PEROXIDE  $NO_2$  300-450K  
 $\mu(T) = 785.544557 - 8.749203T + 3.6259252E-02T^2 - 6.5336018E-05T^3$   
 $+ 4.3577125E-08T^4$   
 $\mu(300) = 13.02$   $\mu(370) = 19.47$   $\mu(450) = 24.09$   
 std error est = 9.4E-02 max error est = 0.2  
300-450K  
 $T(\mu) = 318.245 - 8.8194949\mu + 0.5945482\mu^2$   
 $T(13.02) = 304$   $T(19.47) = 372$   $T(24.09) = 451$   
 - std error est = 2.7 - - - - - max error est = 6.0 -

NITROUS OXIDE  $N_2O$  180-1500K  
 $\mu(T) = -1.4347 + 6.345024E-02T - 3.307219E-05T^2 + 1.3455025E-08T^3$   
 $- 2.4171922E-12T^4$   
 $\mu(180) = 8.99$   $\mu(800) = 34.06$   $\mu(1500) = 52.50$   
 std error est = 2.3E-02 max error est = 0.04  
180-1500K  
 $T(\mu) = 30.57 + 15.037308\mu + 0.1758553\mu^2 + 1.3549377E-03\mu^3$   
 $T(8.99) = 181$   $T(34.06) = 800$   $T(52.50) = 1501$   
 - std error est = 0.8 - - - - - max error est = 2.5 -

OCTAFLUOROCYCLOBUTANE  $C_4F_8$  270-440K

$$\mu(T) = -21.702187 + 0.29705496T - 1.1162856E-03T^2 + 2.126056E-06T^3 - 1.53345928E-09T^4$$

$$\mu(270) = 10.82 \quad \mu(350) = 13.67 \quad \mu(440) = 16.52$$

$$\text{std error est} = 1.2E-02 \quad \text{max error est} = 0.15$$

$$T(\mu) = 51.767 + 13.95912177\mu + 0.574077\mu^2$$

$$T(10.82) = 270 \quad T(13.67) = 350 \quad T(16.52) = 439$$

$$\text{std error est} = 0.6 \quad \text{max error est} = 2.0$$

n-OCTANE  $C_8H_{18}$  300-650K

$$\mu(T) = 0.8324354 + 1.40045E-02T + 8.793765E-06T^2 - 6.8403E-09T^3$$

$$\mu(300) = 5.64 \quad \mu(450) = 8.29 \quad \mu(650) = 11.77$$

$$\text{std error est} = 2.1E-02 \quad \text{max error est} = 0.04$$

$$T(\mu) = -8.63 + 53.900825\mu + 0.167701848\mu^2$$

$$T(5.64) = 301 \quad T(8.29) = 450 \quad T(11.77) = 649$$

$$\text{std error est} = 1.2 \quad \text{max error est} = 3.5$$

OXYGEN  $O_2$  80-2000K

$$\mu(T) = -0.397863 + 8.7605894E-02T - 7.064124E-05T^2 + 4.6287E-08T^3 - 1.690435E-11T^4 + 2.534147E-15T^5$$

$$\mu(80) = 6.18 \quad \mu(1100) = 51.43 \quad \mu(2000) = 73.17$$

$$\text{std error est} = 3.1E-02 \quad \text{max error est} = 0.08$$

$$T(\mu) = 19.02 + 9.362836\mu + 0.185555\mu^2 + 7.899354E-04\mu^3$$

$$T(6.18) = 84 \quad T(51.43) = 1099 \quad T(73.17) = 2007$$

$$\text{std error est} = 1.5 \quad \text{max error est} = 7.0$$

n-PENTANE  $C_5H_{12}$  270-550K

$$\mu(T) = 0.2416119 + 2.307305E-02T - 1.52727E-06T^2$$

$$\mu(270) = 6.36 \quad \mu(400) = 9.23 \quad \mu(550) = 12.47$$

$$\text{std error est} = 8.2E-03 \quad \text{max error est} = 0.02$$

$$T(\mu) = -9.73 + 43.0470668\mu + 0.14747898\mu^2$$

$$T(6.36) = 270 \quad T(9.23) = 400 \quad T(12.47) = 550$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.5$$

PROPANE  $C_3H_8$  270-600K

$$\mu(T) = -0.3543711 + 3.080096E-02T - 6.99723E-06T^2$$

$$\mu(270) = 7.45 \quad \mu(450) = 12.09 \quad \mu(600) = 15.61$$

$$\text{std error est} = 5.9E-03 \quad \text{max error est} = 0.01$$



PROPYLENE  $C_3H_6$  210-360K

$$\mu(T) = -1.1116324 + 0.03663067T - 1.2184874E-05T^2$$

$\mu(210) = 6.04$        $\mu(300) = 8.78$        $\mu(360) = 10.50$   
 std error est = 4.4E-03      max error est = 0.01

210-360K

$$T(\mu) = 36.1 + 25.971212587\mu + 0.4652205\mu^2$$

$T(6.04) = 210$        $T(8.78) = 300$        $T(10.50) = 360$   
 - std error est = 0.2 - - - - - max error est = 1.5

SULFUR DIOXIDE  $SO_2$  200-1250K

$$\mu(T) = -1.141748 + 0.051281456T - 1.3886282E-05T^2 + 2.15266E-09T^3$$

$\mu(200) = 8.58$        $\mu(650) = 26.92$        $\mu(1250) = 45.47$   
 std error est = 3.7E-02      max error est = 0.08

200-1250K

$$T(\mu) = 43.076 + 16.9625\mu + 0.20754597\mu^2$$

$T(8.58) = 204$        $T(26.92) = -50$        $T(45.47) = 1243$   
 - std error est = 2.2 - - - - - max error est = 9.0

TOLUENE  $C_7H_8$  330-550K

$$\mu(T) = -2.2639265 + 3.8294535E-02T - 2.9042466E-05T^2 + 1.6824E-08T^3$$

$\mu(330) = 7.82$        $\mu(450) = 10.62$        $\mu(550) = 12.81$   
 std error est = 2E-02      max error est = 0.04

330-550K

$$T(\mu) = 42.866 + 32.181384\mu + 0.579136617\mu^2$$

$T(7.82) = 330$        $T(10.62) = 450$        $T(12.81) = 550$   
 - std error est = 0.9 - - - - - max error est = 2.0

TRICHLOROFLUOROMETHANE  $CCl_3F$  230-500K  
 (FREON-11)

$$\mu(T) = 4.6926597 + 5.81068E-03T + 6.427175E-05T^2 - 4.712105E-08T^3$$

$\mu(230) = 8.86$        $\mu(400) = 14.28$        $\mu(500) = 17.78$   
 std error est = 6E-03      max error est = 0.01

230-500K

$$T(\mu) = -188.137 + 63.015166\mu - 2.19224063\mu^2 + 4.64365E-02\mu^3$$

$T(8.86) = 230$        $T(14.28) = 400$        $T(17.78) = 500$   
 - std error est = 0.3 - - - - - max error est = 1.5

TRICHLOROTRIFLUOROETHANE  $C_2Cl_3F_3$  230-400K  
 (FREON-113)

$$\mu(T) = 1.5959133 + 3.483849E-02T - 1.8833849E-05T^2$$

$\mu(230) = 8.61$        $\mu(350) = 11.48$        $\mu(400) = 12.52$   
 std error est = 4.9E-03      max error est = 0.01

230-400K

$$T(\mu) = 23.38 + 10.69495544\mu + 1.547242767\mu^2$$

$T(8.61) = 230$        $T(11.48) = 350$        $T(12.52) = 400$   
 - std error est = 0.3 - - - - - max error est = 2.0

TRIFLUOROMETHANE  $\text{CHF}_3$  230-500K

$$\mu(T) = -2.100796 + 6.3910783E-02T - 2.41926655E-05T^2$$

$\mu(230) = 11.32$        $\mu(400) = 19.59$        $\mu(500) = 23.81$   
std error est =  $5.7E-03$       max error est = 0.01

230-500K

$$T(\mu) = 52.246 + 12.98628777\mu + 0.243660334\mu^2$$

$T(11.32) = 230$        $T(19.59) = 400$        $T(23.81) = 500$   
std error est = 0.2      max error est = 1.5

WATER  $\text{H}_2\text{O}$  280-1000K

$$\mu(T) = -3.07514683 + 4.069249E-02T + 5.20585924E-09T^2$$

$\mu(280) = 8.32$        $\mu(650) = 23.38$        $\mu(1000) = 37.62$   
std error est =  $3.3E-03$       max error est = 0.01

280-1000K

$$T(\mu) = 75.57 + 24.574084\mu - 7.7339827E-05\mu^2$$

$T(8.32) = 280$        $T(23.38) = 650$        $T(37.62) = 1000$   
std error est = 0.08      max error est = 1.0

XENON  $\text{Xe}$  120-1500K

$$\mu(T) = 1.89178728 + 6.0506328E-02T + 8.1793523E-05T^2 - 2.051E-07T^3$$
$$+ 2.0164963E-10T^4 - 9.5234E-14T^5 + 1.7662669E-17T^6$$

$\mu(120) = 10.02$        $\mu(800) = 53.65$        $\mu(1500) = 83.33$   
std error est =  $4.2E-02$       max error est = 0.07

120-1500K

$$T(\mu) = 7.02702 + 11.3664655\mu + 0.0360854\mu^2 + 5.165008E-04\mu^3$$

$T(10.02) = 125$        $T(53.65) = 800$        $T(83.33) = 1504$   
std error est = 1.5      max error est = 4.5

APPENDIX D  
TABLE D-I  
SUMMARY OF CONTENTS

THE VIRIAL COEFFICIENTS  
FOR GASEOUS ELEMENTS AND COMPOUNDS

NAME	FORMULA	APP D PAGE
Air (Dry, CO <sub>2</sub> -free)	-	D-1
Argon	Ar	D-1
Carbon Dioxide	CO <sub>2</sub>	D-1
Deuterium	D <sub>2</sub>	D-1
Helium	He	D-2
Hydrogen	H <sub>2</sub>	D-2
Krypton	Kr	D-2
Methane	CH <sub>4</sub>	D-2
Neon	Ne	D-3
Nitrogen	N <sub>2</sub>	D-3
Oxygen	O <sub>2</sub>	D-3
Water Vapor	H <sub>2</sub> O	D-4
'Heavy' Water Vapor	D <sub>2</sub> O	D-4
Xenon	Xe	D-4
TABLE D-II Third Virial Coefficients		D-5

APPENDIX D  
FORMAT EXAMPLE

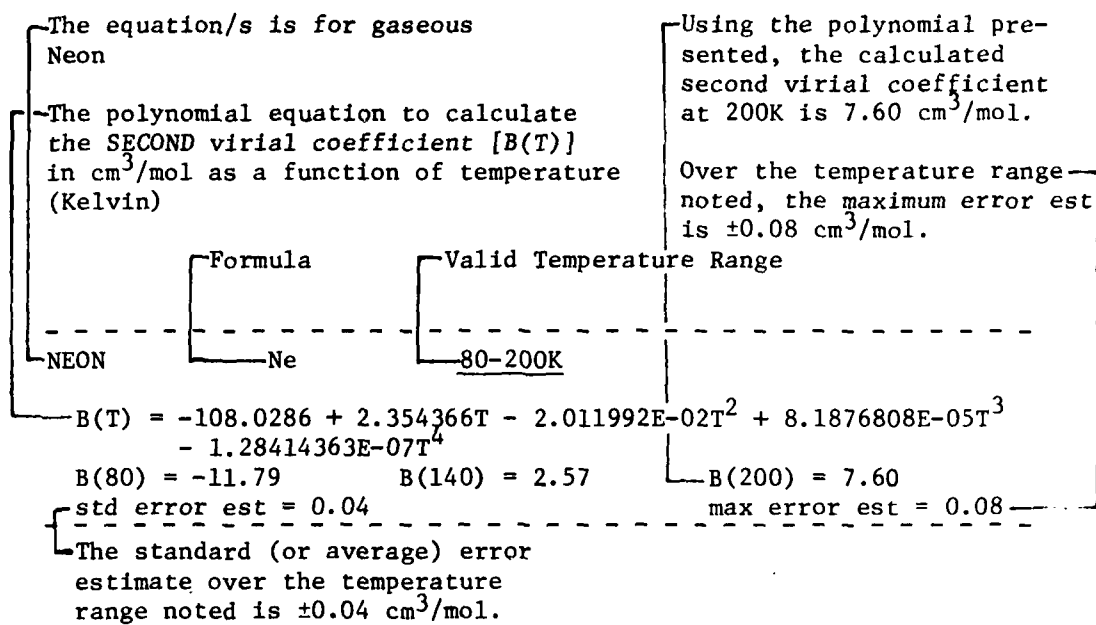


FIGURE D-1

# APPENDIX D

## SECOND VIRIAL COEFFICIENTS FOR GASEOUS ELEMENTS AND COMPOUNDS

AIR (Dry, CO<sub>2</sub>-Free)

100-150K

$$B(T) = -1502.0253 + 31.45448274T - 0.279362289T^2 + 1.1746791E-03T^3 - 1.91779611E-06T^4$$

$$B(100) = -167.30 \quad B(125) = -109.17 \quad B(150) = -75.85$$

$$\text{std error est} = 4.3E-02 \quad \text{max error est} = 0.1$$

150-350K

$$B(T) = -871.7496 + 14.673657T - 0.1155472T^2 + 5.15056917E-04T^3 - 1.32633153E-06T^4 + 1.84350813E-09T^5 - 1.0723866E-12T^6$$

$$B(150) = -75.88 \quad B(250) = -19.77 \quad B(350) = 0.42$$

$$\text{std error est} = 0.2 \quad \text{max error est} = 0.6$$

350-1400K

$$B(T) = -113.0307 + 0.6191348T - 1.1961097E-03T^2 + 1.2117027E-06T^3 - 6.19795E-10T^4 + 1.2599233E-13T^5$$

$$B(350) = 0.53 \quad B(800) = 24.75 \quad B(1400) = 31.21$$

$$\text{std error est} = 0.092 \quad \text{max error est} = 0.35$$

ARGON

Ar

80-250K

$$B(T) = -2602.5842 + 71.103308T - 0.8814188T^2 + 5.9930164E-03T^3 - 2.3043749E-05T^4 + 4.704073E-08T^5 - 3.96383723E-11T^6$$

$$\text{std error est} = 0.35 \quad B(200) = -48.36 \quad \text{max error est} = 0.9$$

250-1500K

$$B(T) = -195.60895 + 1.2604989T - 3.370398E-03T^2 + 4.9626165E-06T^3 - 4.0932672E-09T^4 + 1.76812575E-12T^5 - 3.1081026E-16T^6$$

$$B(250) = -27.93 \quad B(700) = 15.23 \quad B(1500) = 24.79$$

$$\text{std error est} = 0.16 \quad \text{max error est} = 0.4$$

CARBON DIOXIDE

CO<sub>2</sub>

250-1000K

$$B(T) = -1495.9175 + 11.9968622T - 4.31032436E-02T^2 + 8.501674E-05T^3 - 9.4651135E-08T^4 + 5.57671E-11T^5 - 1.3516095E-14T^6$$

$$B(250) = -180.84 \quad B(700) = -1.08 \quad B(1000) = 14.31$$

$$\text{std error est} = 0.35 \quad \text{max error est} = 1.0$$

DEUTERIUM

D<sub>2</sub>

85-420K

$$B(T) = -104.569 + 2.1780589T - 1.84434317E-02T^2 + 8.7373826E-05T^3 - 2.36196123E-07T^4 + 3.3976588E-10T^5 - 2.0138934E-13T^6$$

$$B(85) = -9.93 \quad B(300) = 13.66 \quad B(420) = 15.45$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 0.2$$

HELIUM                      He                      20-200K  

$$B(T) = -34.55944 + 2.7175236T - 7.238207E-02T^2 + 1.0230434E-03T^3$$

$$- 7.80158414E-06T^4 + 3.01349506E-08T^5 - 4.60368796E-11T^6$$

$$B(20) = -2.13 \quad B(100) = 11.57 \quad B(200) = 12.30$$

$$\text{std error est} = 0.14 \quad \text{max error est} = 0.25$$
  
275-1400K  

$$B(T) = 16.797 - 2.974167E-02T + 5.9985787E-05T^2 - 6.536E-08T^3$$

$$+ 3.4774704E-11T^4 - 7.17233967E-15T^5$$

$$B(275) = 11.98 \quad B(600) = 10.38 \quad B(1400) = 8.40$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.09$$


---

 HYDROGEN                      H<sub>2</sub>                      25-100K  

$$B(T) = -552.3468 + 37.9672515T - 1.2583684T^2 + 2.3661885E-02T^3$$

$$- 2.55707365E-04T^4 + 1.479355E-06T^5 - 3.547909E-09T^6$$

$$B(25) = -106.23 \quad B(50) = -33.48 \quad B(100) = -2.52$$

$$\text{std error est} = 0.1 \quad \text{max error est} = 0.25$$
  
120-420K  

$$B(T) = -28.6784 + 0.2390086T + 1.6559E-03T^2 - 2.0165055E-05T^3$$

$$+ 7.74730172E-08T^4 - 1.3371575E-10T^5 + 8.80146735E-14T^6$$

$$B(120) = 2.00 \quad B(350) = 15.32 \quad B(420) = 16.11$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.1$$


---

 KRYPTON                      Kr                      125-200K  

$$B(T) = -3767.455 + 79.33045T - 0.7427849T^2 + 3.65588424E-03T^3$$

$$- 9.2488483E-06T^4 + 9.5193755E-09T^5$$

$$B(125) = -284.18 \quad B(160) = -178.36 \quad B(200) = -117.39$$

$$\text{std error est} = 0.03 \quad \text{max error est} = 0.1$$
  
200-400K  

$$B(T) = -1195.697 + 14.577052T - 8.36262E-02T^2 + 2.714544E-04T^3$$

$$- 5.095532E-07T^4 + 5.16988543E-10T^5 - 2.19801246E-13T^6$$

$$B(200) = -117.62 \quad B(300) = -51.00 \quad B(400) = -22.89$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.1$$
  
400-1500K  

$$B(T) = -285.26 + 1.490866T - 3.3921494E-03T^2 + 4.3542916E-06T^3$$

$$- 3.1988343E-09T^4 + 1.253671E-12T^5 - 2.030971E-16T^6$$

$$B(400) = -22.87 \quad B(800) = 13.17 \quad B(1500) = 27.00$$

$$\text{std error est} = 0.05 \quad \text{max error est} = 0.1$$


---

 METHANE                      CH<sub>4</sub>                      110-200K  

$$B(T) = -4564.8011 + 108.37155T - 1.1344657T^2 + 6.2125655E-03T^3$$

$$- 1.742442E-05T^4 + 1.9820625E-08T^5$$

$$B(110) = -333.94 \quad B(160) = -161.93 \quad B(200) = -105.07$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.1$$

METHANE (continued) 200-400K  
 $B(T) = -1161.958 + 14.527312T - 8.4895E-02T^2 + 2.7964493E-04T^3$   
 $- 5.300204E-07T^4 + 5.396463E-10T^5 - 2.28570436E-13T^6$   
 $B(200) = -105.11$   $B(300) = -42.35$   $B(400) = -15.73$   
std error est = 0.04 max error est = 0.07

400-1500K  
 $B(T) = -263.0827 + 1.39774T - 3.15891435E-03T^2 + 4.03489206E-06T^3$   
 $- 2.954616E-09T^4 + 1.155816E-12T^5 - 1.87089616E-16T^6$   
 $B(400) = -15.75$   $B(900) = 22.15$   $B(1500) = 31.90$   
std error est = 0.06 max error est = 0.15

---

NEON Ne 80-200K  
 $B(T) = -108.0286 + 2.354366T - 2.011992E-02T^2 + 8.1876808E-05T^3$   
 $- 1.28414363E-07T^4$   
 $B(80) = -11.79$   $B(140) = 2.57$   $B(200) = 7.60$   
std error est = 0.04 max error est = 0.08

200-1000K  
 $B(T) = -18.52 + 0.253489T - 8.9773E-04T^2 + 1.76985156E-06T^3$   
 $- 1.98866447E-09T^4 + 1.1902623E-12T^5 - 2.9438917E-16T^6$   
 $B(200) = 7.61$   $B(600) = 13.77$   $B(1000) = 14.30$   
std error est = 0.03 max error est = 0.05

---

NITROGEN  $N_2$  100-150K  
 $B(T) = -1934.0 + 49.775958T - 0.5771643T^2 + 3.5473302E-03T^3$   
 $- 1.12452359E-05T^4 + 1.45225962E-08T^5$   
 $B(100) = -159.85$   $B(125) = -103.84$   $B(150) = -71.41$   
std error est = 0.05 max error est = 0.09

150-325K  
 $B(T) = -1038.812 + 19.7330247T - 0.17557828T^2 + 8.834965E-04T^3$   
 $- 2.567272E-06T^4 + 4.0252916E-09T^5 - 2.6402379E-12T^6$   
 $B(150) = -71.65$   $B(230) = -23.12$   $B(325) = -0.36$   
std error est = 0.04 max error est = 0.09

325-1400K  
 $B(T) = -156.96 + 1.0434304T - 2.717715E-03T^2 + 3.9752575E-06T^3$   
 $- 3.3108834E-09T^4 + 1.462975E-12T^5 - 2.65735587E-16T^6$   
 $B(325) = -0.39$   $B(800) = 27.37$   $B(1400) = 33.50$   
std error est = 0.05 max error est = 0.1

---

OXYGEN  $O_2$  100-200K  
 $B(T) = -2793.674 + 78.48548T - 1.0166435T^2 + 7.34716756E-03T^3$   
 $- 3.052873E-05T^4 + 6.8392904E-08T^5 - 6.4137155E-11T^6$   
 $B(100) = -197.47$   $B(150) = -90.79$   $B(200) = -49.99$   
std error est = 0.035 max error est = 0.08

OXYGEN (continued)      200-400K

$$B(T) = -499.657 + 5.4925876T - 2.7027447E-02T^2 + 7.1352086E-05T^3$$

$$- 9.750388E-08T^4 + 5.4294996E-11T^5$$

B(200) = -50.05      B(300) = -15.69      B(400) = -0.60  
std error est = 0.03      max error est = 0.05

400-1400K

$$B(T) = -165.1965 + 1.0063385T - 2.541077E-03T^2 + 3.630033E-06T^3$$

$$- 2.9679937E-09T^4 + 1.29213468E-12T^5 - 2.318393E-16T^6$$

B(400) = -0.61      B(900) = 21.01      B(1400) = 25.90  
std error est = 0.02      max error est = 0.05

---

WATER VAPOR      H<sub>2</sub>O      430-720K

$$B(T) = -39636.088 + 319.317424T - 1.039708598T^2 + 1.69863388E-03T^3$$

$$- 1.38836432E-06T^4 + 4.53516028E-10T^5$$

B(430) = -316.78      B(530) = -147.27      B(720) = -96.19  
std error est = 0.6      max error est = 1.3

---

'HEAVY' WATER VAPOR      D<sub>2</sub>O      430-720K

$$B(T) = -40275.7499 + 324.5981063T - 1.057308467T^2 + 1.7280874E-03T^3$$

$$- 1.41303458E-06T^4 + 4.6177338E-10T^5$$

B(430) = -320.24      B(550) = -133.22      B(720) = -56.19  
std error est = 0.6      max error est = 1.5

---

XENON      Xe      220-500K

$$B(T) = -2694.3436 + 32.305283T - 0.181532587T^2 + 5.744002E-04T^3$$

$$- 1.04996174E-06T^4 + 1.03791638E-09T^5 - 4.30480244E-13T^6$$

B(200) = -230.65      B(400) = -69.84      B(550) = -31.53  
std error est = 0.05      max error est = 0.1

500-1500K

$$B(T) = -490.2594 + 2.20020277T - 4.4278794E-03T^2 + 5.059897E-06T^3$$

$$- 3.3321925E-09T^4 + 1.17879258E-12T^5 - 1.735293E-16T^6$$

B(500) = -38.78      B(1000) = 15.03      B(1500) = 30.09  
std error est = 0.05      max error est = 0.1

---



TABLE D-II

THE THIRD VIRIAL COEFFICIENTS OF GASEOUS ELEMENTS AND COMPOUNDS*														
T, K	He	Ne	Ar	Kr	Xe	N <sub>2</sub>	O <sub>2</sub>	Air	H <sub>2</sub>	D <sub>2</sub>	H <sub>2</sub> O	D <sub>2</sub> O	CO <sub>2</sub>	CH <sub>4</sub>
25									14					
30									16					
35									14.3					
40									12.1					
45									10.7					
50									9.6					
55									8.9					
60	2.7	4							8.4					
70	2.5	4							7.4					
80	2.4	4	7						6.9					
90	2.3	4	9						6.4					
100	2.2	4	12						6.1	6				
110	2.1	3	16						5.9	5				
120	2.0	3	20						5.7	5				
130	1.9	3	23						5.5	5				
140	1.8	3	25					28	5.4	5				
150	1.7	3	23					26	5.3	5				
160	1.6	3	22			26	23	24	5.2	5				
180	1.5	3	20			21	20	21	5.0	5				
200	1.3	3	18			19	17	19	4.8	5				
220	1.2	3	16	33		17	15	18	4.6	5				
240	1.1	3	15	30		16	13	17	4.5	5				
260	1.1	3	13	28		15	12	16	4.4	5				
273	1.1	3	12	27	62	15	11	15	4.2	5			57	29
280	1.0	3	12	26	59	15	11	15	4.1	5			56	28
300	1.0	2	11	24	54	14	10	15	3.9	5			52	26
320	1.0	2	11	23	50	14		14	3.6	5			49	25
340	.9	2	10	21	46	14		14	3.4	5			45	24
360	.8	2	9	20	41	13			3.2	5			42	22
380	.8	2	9	19	36	13			3.0	4			38	19
400	.7	2	9	18	34	13			2.9	4			36	17
420	.7		9	18	32	12				3			32	16
440			8	17	30	12								15
460			8	16	28	12								14
480			8	16	26	12								14
500			7	15	24	12					-100	-150		14
525			7	15	22						-53	-64		12
550			7	14	20						-17	-20		12
575			7	14	18						+2	0		11
600			7	13							9	8		11
650				13							12	12		
700				12							10	12		

\*Units: 100 cm<sup>6</sup>/mol<sup>2</sup>

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